Geza Fogarasi

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

56 papers	6,699 citations	31 h-index	56 g-index
56 ext. papers	6,880 ext. citations	4.2 avg, IF	5.18 L-index

#	Paper	IF	Citations
56	Quantum chemical MP2 results on some hydrates of cytosine: binding sites, energies and the first hydration shell. *Physical Chemistry Chemical Physics*, **2015**, 17, 29880-90	3.6	10
55	Benchmark studies on the building blocks of DNA. 2. Effect of biological environment on the electronic excitation spectrum of nucleobases. *Journal of Physical Chemistry A*, **2012**, 116, 8851-60	2.8	31
54	Tautomers of cytosine and their excited electronic states: a matrix isolation spectroscopic and quantum chemical study. *Physical Chemistry Chemical Physics*, **2011**, 13, 6799-807	3.6	73
53	Studies on tautomerism: Benchmark quantum chemical calculations on formamide and formamidine. *Journal of Molecular Structure*, **2010**, 978, 257-262	3.4	19
52	Reinterpretation of the UV spectrum of cytosine: only two electronic transitions?. *ChemPhysChem*, **2009**, 10, 1603-6	3.2	27
51	Water-mediated tautomerization of cytosine to the rare imino form: An ab initio dynamics study. *Chemical Physics*, **2008**, 349, 204-209	2.3	26
50	Fock matrix dynamics. *Chemical Physics Letters*, **2004**, 386, 272-278	2.5	80
49	The interaction between cytosine tautomers and water: an MP2 and coupled cluster electron correlation study. *Chemical Physics Letters*, **2002**, 356, 383-390	2.5	42
48	Relative Stabilities of Three Low-Energy Tautomers of Cytosine: A Coupled Cluster Electron Correlation Study. *Journal of Physical Chemistry A*, **2002**, 106, 1381-1390	2.8	108
47	Gas-Phase Molecular Structure of MBBA (4-Methoxybenzylidene-4□h-butylaniline), a Mesogen, by Electron Diffraction Combined with ab Initio Calculations. *Journal of Physical Chemistry A*, **1999**, 103, 3054-3061	2.8	25
46	Isomers of Manganese Tetracarbonyl Hydride: A Density Functional Study of Structure and Vibrational Spectra. *Organometallics*, **1999**, 18, 5245-5251	3.8	5
45	Molecular Structure of p-Azoxyanisole, a Mesogen, Determined by Gas-Phase Electron Diffraction Augmented by ab Initio Calculations. *Journal of Physical Chemistry A*, **1998**, 102, 2080-2086	2.8	28
44	An efficient direct method for geometry optimization of large molecules in internal coordinates. *Journal of Chemical Physics*, **1998**, 109, 6571-6576	3.9	40
43	High-Level Electron Correlation Calculations on Formamide and the Resonance Model. *Journal of Physical Chemistry A*, **1997**, 101, 1400-1408	2.8	118
42	Recent developments in the method of SQM force fields with application to 1-methyladenine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **1997**, 53, 1211-1224	4.4	19
41	High-level electron correlation calculations on some tautomers of cytosine. *Journal of Molecular Structure*, **1997**, 413-414, 271-278	3.4	53
40	Theoretical prediction of the electronic excited states and resonance Raman intensities in formamide from coupled cluster calculations. *Chemical Physics Letters*, **1997**, 270, 406-412	2.5	25

39	Quantum chemical coupled cluster study of the structure and spectra of the ground and first excited states of the ketenyl radical. *Chemical Physics Letters*, **1996**, 263, 91-99	2.5	40
38	Scaled quantum mechanical (SQM) force field and vibrational assignment for styrene. *Computational and Theoretical Chemistry*, **1994**, 306, 293-311		28
37	Effect of nondynamical electron correlation on the geometries of conjugated .pi.-systems. *The Journal of Physical Chemistry*, **1993**, 97, 4036-4043		34
36	The Use of Natural Coordinates in Molecular Geometry Optimizations **1993**, 375-390		1
35	A priori results for molecular geometry, scaled quantum mechanical (SQM) force field, and vibrational spectra of pyridazine. *The Journal of Physical Chemistry*, **1993**, 97, 1356-1363		12
34	Building a database of force constants based on scaled ab initio (SQM) results. I. Chlorobenzenes. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1993**, 49, 1499-1514		14
33	The calculation of ab initio molecular geometries: efficient optimization by natural internal coordinates and empirical correction by offset forces. *Journal of the American Chemical Society*, **1992**, 114, 8191-8201	16.4	852
32	Geometry optimization in redundant internal coordinates. *Journal of Chemical Physics*, **1992**, 96, 2856-2860	3.9	272
31	Theoretical prediction of vibrational spectra. The a priori scaled quantum mechanical (SQM) force field and vibrational spectra of pyrimidine. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1992**, 48, 111-119		50
30	The geometries of chlorobenzenes as obtained from ab initio calculations empirically corrected by offset forces. *Computational and Theoretical Chemistry*, **1992**, 277, 147-160		2
29	Ab initio quantum mechanical calculation of the nitrogen chemical-shift tensor of the imine moiety of benzylideneaniline and analogs of all-trans-retinylidenebutylimine. *Journal of Magnetic Resonance*, **1992**, 96, 154-158		3
28	Ab initio prediction of vibrational spectra: A database approach. *Vibrational Spectroscopy*, **1990**, 1, 159-165	2.1	68
27	An ab initio study of the structure and vibrational spectra of allyl and 1,4-pentadienyl radicals. *Journal of Chemical Physics*, **1990**, 93, 1246-1256	3.9	42
26	Theoretical prediction of the vibrational spectrum geometry and scaled quantum mechanical force field for phenylacetylene. *The Journal of Physical Chemistry*, **1989**, 93, 7644-7651		32
25	Scaled quantum mechanical (SQM) force field and theoretical vibrational spectrum for benzonitrile. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1989**, 45, 845-854		59
24	Theoretical prediction of vibrational spectra. Scaled quantum mechanical (SQM) force field for fluorobenzene. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1988**, 44, 1067-1077		37
23	On the use of scaled quantum mechanical force fields for predicting quartic centrifugal distortion constants. *Journal of Chemical Physics*, **1988**, 89, 7646-7648	3.9	12
22	Scaled quantum mechanical (SQM) force field and vibrational assignment for hexatriene. *Computational and Theoretical Chemistry*, **1987**, 151, 341-354		32

21	Determination of an isotope-independent puckering potential function of oxetane. *Journal of Molecular Spectroscopy*, **1987**, 126, 1-12	1.3	9
20	Quantum chemical calculation of force constants and vibrational spectra. *Journal of Molecular Structure*, **1986**, 141, 145-152	3.4	31
19	Scaled quantum mechanical (SQM) force field and vibrational assignment for cyclohexane. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1985**, 41, 425-433		17
18	Theoretical prediction of vibrational spectra: The out-of-plane force field and vibrational spectra of pyridine. *Journal of Molecular Spectroscopy*, **1985**, 114, 445-453	1.3	34
17	A comparative ab initio study of amides. *Computational and Theoretical Chemistry*, **1985**, 133, 105-123		48
16	Theoretical prediction of vibrational spectra. 1. The in-plane force field and vibrational spectra of pyridine. *Journal of the American Chemical Society*, **1984**, 106, 2765-2769	16.4	131
15	Combination of theoretical ab initio and experimental information to obtain reliable harmonic force constants. Scaled quantum mechanical (QM) force fields for glyoxal, acrolein, butadiene, formaldehyde, and ethylene. *Journal of the American Chemical Society*, **1983**, 105, 7037-7047	16.4	1350
14	Theoretical equilibrium geometry, vibrational frequencies and the first electronic transition energy of HCC. *Molecular Physics*, **1983**, 50, 139-151	1.7	33
13	Ab initio study of the vibrational spectrum and geometry of oxetane. Interpretation of the vibrational spectra. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1983**, 39, 761-769		17
12	Force field and vibrational assignment for cyclobutane from a combination of ab initio calculations and experimental data. *Computational and Theoretical Chemistry*, **1982**, 89, 1-13		32
11	Force field, dipole moment derivatives, and vibronic constants of benzene from a combination of experimental and ab initio quantum chemical information. *Journal of Chemical Physics*, **1981**, 74, 3999-4014	3.9	415
10	The general valence force field of perchloryl fluoride. *Spectrochimica Acta Part A: Molecular Spectroscopy*, **1981**, 37, 549-556		9
9	The molecular structure of toluene. *Journal of Molecular Structure*, **1980**, 66, 281-287	3.4	68
8	Ab inttio structural analysis of some saturated 3- and 4-membered rings. *Journal of Molecular Structure*, **1980**, 62, 259-273	3.4	70
7	CNDO/2 force field and normal coordinate analysis of 2,6-dimethyl-1,5-dehydro-1,2,3-triazolo-[2,1a]-1,2,3-triazole. *Journal of Molecular Structure*, **1979**, 56, 277-282	3.4	2
6	The geometry of some amides obtained from ab initio calculations. *Journal of Molecular Structure*, **1979**, 57, 259-270	3.4	73
5	Systematic ab initio gradient calculation of molecular geometries, force constants, and dipole moment derivatives. *Journal of the American Chemical Society*, **1979**, 101, 2550-2560	16.4	1942
4	Ab initio Hartree-Fock calculation of the force constants and geometry of HNF2 and H2NF. *Molecular Physics*, **1977**, 33, 1565-1570	1.7	36

3	The flexibility of the cyclotrisiloxane ring as discussed in a strongly anharmonic vibrational model. *Journal of Molecular Structure*, **1977**, 41, 139-147	3.4	2
2	Prediction of vibrational spectra by the CNDO/2 force method. *Journal of Molecular Structure*, **1977**, 39, 275-280	3.4	55
1	The in-plane force field of nitryl fluoride. *Molecular Physics*, **1976**, 32, 169-176	1.7	6