Filip Uhlik

List of Publications by Citations

179 papers	2,441 citations	27 h-index	37 g-index
190 ext. papers	2,686 ext. citations	3.3 avg, IF	4.88 L-index

#	Paper	IF	Citations
179	Computing relative stabilities of metallofullerenes by Gibbs energy treatments. *Theoretical Chemistry Accounts*, **2007**, 117, 315-322	1.9	94
178	Enhanced relaxation and intermixing in Ge islands grown on pit-patterned Si(001) substrates. *Physical Review Letters*, **2009**, 102, 025502	7.4	78
177	AM1 computations on seven isolated-pentagon-rule isomers of C80. *Chemical Physics Letters*, **1995**, 246, 66-72	2.5	67
176	Enthalpy–entropy interplay for C36 cages: B3LYP/6-31G* calculations. *Journal of Chemical Physics*, **2000**, 113, 4933	3.9	65
175	La2@C72 and Sc2@C72: computational characterizations. *Journal of Physical Chemistry A*, **2006**, 110, 2231-4	2.8	54
174	Electron pairing and chemical bonds. On the accuracy of the electron pair model of chemical bond. *Computational and Theoretical Chemistry*, **1997**, 391, 159-168		51
173	Computational modeling of the elemental catalysis in the Stone–Wales fullerene rearrangements. *Journal of Organometallic Chemistry*, **2000**, 599, 57-61	2.3	51
172	Modeling of Ionization and Conformations of Starlike Weak Polyelectrolytes. *Macromolecules*, **2014**, 47, 4004-4016	5.5	48
171	Polyelectrolyte Behavior of Polystyrene-block-poly(methacrylic acid) Micelles in Aqueous Solutions at Low Ionic Strength. *Macromolecules*, **2004**, 37, 10141-10154	5.5	48
170	Computed structure and energetics of La@C60. *International Journal of Quantum Chemistry*, **2005**, 104, 272-277	2.1	42
169	Local pH and effective pK of weak polyelectrolytes - insights from computer simulations. *Physical Chemistry Chemical Physics*, **2017**, 19, 14376-14387	3.6	41
168	Simulations of ionization equilibria in weak polyelectrolyte solutions and gels. *Soft Matter*, **2019**, 15, 1155-1185	3.6	41
167	Intrinsic Viscosity of Cyclic Polystyrene. *Macromolecules*, **2017**, 50, 7770-7776	5.5	39
166	Facile Synthesis of an Extensive Family of Sc2O@C2n (n = 35–47) and Chemical Insight into the Smallest Member of Sc2O@C2(7892)–C70. *Journal of Physical Chemistry C*, **2014**, 118, 28883-28889	3.8	39
165	Hiding and recovering electrons in a dimetallic endohedral fullerene: air-stable products from radical additions. *Journal of the American Chemical Society*, **2015**, 137, 232-8	16.4	38
164	MPWB1K calculations of stepwise encapsulations: Lix@C60. *Chemical Physics Letters*, **2008**, 463, 121-123	2.5	36
163	Experimental Study of Hydrophobically Modified Amphiphilic Block Copolymer Micelles Using Light Scattering and Nonradiative Excitation Energy Transfer. *Macromolecules*, **2002**, 35, 9487-9496	5.5	35

162	Computed structures of two known Yb@C74 isomers. *Journal of Physical Chemistry A*, **2006**, 110, 12860-3	2.8	34
161	Sm@C2v(19138)-C76: A Non-IPR Cage Stabilized by a Divalent Metal Ion. *Inorganic Chemistry*, **2015**, 54, 4243-8	5.1	32
160	Isolation and Crystallographic Characterization of the Labile Isomer of Y@C82 Cocrystallized with Ni(OEP): Unprecedented Dimerization of Pristine Metallofullerenes. *Angewandte Chemie - International Edition*, **2016**, 55, 9234-8	16.4	32
159	La2@C(s)(17,490)-C76: a new non-IPR dimetallic metallofullerene featuring unexpectedly weak metal-pentalene interactions. *Chemistry - A European Journal*, **2013**, 19, 17125-30	4.8	31
158	Computing enthalpy□ntropy interplay for isomeric fullerenes. *International Journal of Quantum Chemistry*, **2004**, 99, 640-653	2.1	31
157	Ab Initio SCF Nonlinear Pair Population Analysis. A New Means of Detection and Localization of Multicenter Bonding. *Inorganic Chemistry*, **1997**, 36, 5363-5368	5.1	29
156	Intermixing in heteroepitaxial islands: fast, self-consistent calculation of the concentration profile minimizing the elastic energy. *New Journal of Physics*, **2008**, 10, 083039	2.9	29
155	Polyelectrolyte shells of copolymer micelles in aqueous solutions: a Monte Carlo study. *Journal of Chemical Physics*, **2004**, 121, 2367-75	3.9	29
154	Computing the relative gas-phase populations of C60 and C70: beyond the traditional delta H(fo),298 scale. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 216-21	2.8	28
153	Synthesis and photophysical properties of □bis(terpyridine)oligothiophenes. *Tetrahedron*, **2011**, 67, 75-79	2.4	27
152	Evidence for fullerenes in solid bitumen from pillow lavas of Proterozoic age from M□ov (Bohemian Massif, Czech Republic). *Geochimica Et Cosmochimica Acta*, **2003**, 67, 1495-1506	5.5	27
151	Isomeric ScO@C Related by a Single-Step Stone-Wales Transformation: Key Links in an Unprecedented Fullerene Formation Pathway. *Inorganic Chemistry*, **2016**, 55, 11354-11361	5.1	27
150	Computed stabilities in metallofullerene series: Al@C82, Sc@C82, Y@C82, and La@C82. *International Journal of Quantum Chemistry*, **2011**, 111, 2712-2718	2.1	26
149	Temperature dependence of the Gibbs energy ordering of isomers of chlorine oxide (Cl2O2). *The Journal of Physical Chemistry*, **1991**, 95, 5432-5434		25
148	Mg@C72 MNDO/d evaluation of the isomeric composition. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 252-5	2.8	24
147	Isolation and Structural Characterization of Er@ C(9)-C and Er@ C (6)-C: Regioselective Dimerization of a Pristine Endohedral Metallofullerene Induced by Cage Symmetry. *Inorganic Chemistry*, **2019**, 58, 2177-2182	5.1	24
146	Computational evaluation of the relative production yields in the X@C74 series (X=Ca, Sr, Ba). *Chemical Physics Letters*, **2007**, 440, 259-262	2.5	23
145	Tuning intramolecular electron and energy transfer processes in novel conjugates of La2@C80 and electron accepting subphthalocyanines. *Chemical Communications*, **2015**, 51, 330-3	5.8	22

144	Computational modelling for the clustering degree in the saturated steam and the water-containing complexes in the atmosphere. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **2006**, 97, 415-423	2.1	22
143	Zeolite (In)Stability under Aqueous or Steaming Conditions. *Advanced Materials*, **2020**, 32, e2003264	24	22
142	Charge-controlled nano-structuring in partially collapsed star-shaped macromolecules. *Soft Matter*, **2016**, 12, 4846-52	3.6	22
141	HoO@C: HoO Cluster Expands within a Small Non-IPR Fullerene Cage of C(13333)-C. *Inorganic Chemistry*, **2019**, 58, 4774-4781	5.1	20
140	Silver(i) complexes with 1Ꝕ(diphenylphosphino)-1-cyanoferrocene: the art of improvisation in coordination. *Dalton Transactions*, **2016**, 45, 10655-71	4.3	20
139	Nonradiative Excitation Energy Transfer in Hydrophobically Modified Amphiphilic Block Copolymer Micelles. Theoretical Model and Monte Carlo Simulations. *Macromolecules*, **2002**, 35, 9497-9505	5.5	20
138	Endohedrally stabilized C70 isomer with fused pentagons characterized by crystallography. *Dalton Transactions*, **2016**, 45, 8142-8	4.3	20
137	The Unanticipated Dimerization of Ce@C (9)-C upon Co-crystallization with Ni(octaethylporphyrin) and Comparison with Monomeric M@C (9)-C (M = La, Sc, and Y). *Chemistry - A European Journal*, **2016**, 22, 18115-18122	4.8	19
136	Structural and electrochemical studies of Sm@D3h-C74 reveal a weak metal-cage interaction and a small band gap species. *Nanoscale*, **2013**, 5, 10409-13	7.7	19
135	Popular C82 fullerene cage encapsulating a divalent metal ion Sm(2+): structure and electrochemistry. *Inorganic Chemistry*, **2015**, 54, 2103-8	5.1	19
134	Computed structures and relative stabilities of Be@C74. *International Journal of Quantum Chemistry*, **2007**, 107, 2494-2498	2.1	18
133	A Monte Carlo study of shells of hydrophobically modified amphiphilic copolymer micelles in polar solvents. *Journal of Chemical Physics*, **2003**, 118, 11258-11264	3.9	18
132	Calculations of Metallofullerene Yields. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 2233-2239	0.3	17
131	Computed stabilization for a giant fullerene endohedral: Y2C2@C1(1660)-C108. *Chemical Physics Letters*, **2018**, 710, 147-149	2.5	15
130	Excited electronic states and relative stabilities of C80 isomers. *International Journal of Quantum Chemistry*, **2006**, 106, 2222-2228	2.1	15
129	Enhancement of fullerene stabilities from excited electronic states. *Computing Letters*, **2005**, 1, 304-312		15
128	C 78 IPR fullerenes: Computed B3LYP/6-31G*//HF/3-21G temperature-dependent relative concentrations. *European Physical Journal D*, **2001**, 16, 349-352	1.3	15
127	Synthesis and non-conventional structure of square-planar Pd(ii) and Pt(ii) complexes with an N,C,N-chelated stibinidene ligand. *Dalton Transactions*, **2018**, 47, 5812-5822	4.3	14

126	Synthesis, Crystal Structures, and Electrochemical Behavior of Fe2Ru Heterobimetallic Complexes with Bridged Metallocene Units. *Organometallics*, **2014**, 33, 5020-5032	3.8	14
125	Eu@C: Computed Comparable Populations of Two Non-IPR Isomers. *Molecules*, **2017**, 22,	4.8	14
124	Computations on three isomers of La@C74. *International Journal of Quantum Chemistry*, **2008**, 108, 2636-2640	2.2	14
123	Reaction of Zirconacyclopentadienes with Ethynylferrocenes. *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 351-364		14
122	Computational studies of atmospheric chemistry species. *Computational and Theoretical Chemistry*, **1993**, 282, 271-275		14
121	Local pH and Effective pK of a Polyelectrolyte Chain: Two Names for One Quantity?. *ACS Macro Letters*, **2018**, 7, 1243-1247	6.6	14
120	Adamantylidene Addition to M N@I -C (M=Sc, Lu) and Sc N@D -C : Synthesis and Crystallographic Characterization of the [5,6]-Open and [6,6]-Open Adducts. *Chemistry - A European Journal*, **2017**, 23, 6552-6561	4.8	13
119	Calculations of the water-dimer encapsulations into C84. *Fullerenes Nanotubes and Carbon Nanostructures*, **2016**, 24, 1-7	1.8	13
118	A computational characterization of CO@C60. *Fullerenes Nanotubes and Carbon Nanostructures*, **2017**, 25, 624-629	1.8	13
117	Water-Dimer Stability and Its Fullerene Encapsulations. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 959-964	0.3	13
116	Synthesis of phosphinoferrocene amides and thioamides from carbamoyl chlorides and the structural chemistry of Group 11 metal complexes with these mixed-donor ligands. *Dalton Transactions*, **2015**, 44, 3092-108	4.3	13
115	Computations on C84O: thermodynamic, kinetic and photochemical stability. *Computational and Theoretical Chemistry*, **2004**, 684, 129-133		13
114	A Computational Treatment of 35 IPR Isomers of C88. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2000**, 8, 417-432		13
113	Evaluation of the relative stabilities of two non-IPR isomers of Sm@C76. *Fullerenes Nanotubes and Carbon Nanostructures*, **2016**, 24, 339-344	1.8	12
112	Calculated relative yields for Sc2S@C82 and Y2S@C82. *Theoretical Chemistry Accounts*, **2011**, 130, 549-554	1.9	12
111	Li(x)@C(60): Calculations of the encapsulation energetics and thermodynamics. *International Journal of Molecular Sciences*, **2008**, 9, 1841-50	6.3	12
110	HoO@C: Crystallographic Evidence Showing Linear Metallic Oxide Cluster Encapsulated in IPR Fullerene Cage of (51591)-C. *Inorganic Chemistry*, **2019**, 58, 10905-10911	5.1	11
109	Antimony(i) -jPd(ii) complexes with the (Et5Sb)Pd coordination framework. *Dalton Transactions*, **2019**, 48, 11912-11920	4.3	11

108	Computed Relative Populations of D2 (22)-C84 Endohedrals with Encapsulated Monomeric and Dimeric Water. *ChemPhysChem*, **2016**, 17, 1109-11	3.2	11
107	Comparing the reactivity of isomeric phosphinoferrocene nitrile and isocyanide in Pd(ii) complexes: synthesis of simple coordination compounds vs. preparation of P-chelated insertion products and Fischer-type carbenes. *Dalton Transactions*, **2018**, 47, 16082-16101	4.3	11
106	Stability calculations for Eu@C74 isomers. *International Journal of Quantum Chemistry*, **2013**, 113, 729-733	2.1	10
105	Stability computations for isomers of La@C(n) (n = 72, 74, 76). *Molecules*, **2012**, 17, 13146-56	4.8	10
104	Electronic excited states and stabilities of fullerenes: Isomers of C78 and Mg@C72. *International Journal of Quantum Chemistry*, **2004**, 100, 610-616	2.1	10
103	Quantum-Chemical Calculations of Model Systems of Interest in Fullerene-Based Superconductivity. *Journal of Low Temperature Physics*, **2003**, 131, 1259-1263	1.3	10
102	C94 IPR isomeric set: large-scale computations of relative stabilities based on the Gibbs function. *Computational and Theoretical Chemistry*, **2003**, 630, 205-213		10
101	Computations of model narrow nanotubes closed by fragments of smaller fullerenes and quasi-fullerenes. *Journal of Molecular Graphics and Modelling*, **2003**, 21, 517-22	2.8	10
100	Two C60O Structures and Their Relative Stabilities: AM1 Computations. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1993**, 1, 537-546		10
99	AM1 computed relative equilibrium populations of the ( ) and ( ) methanobuckminsterfullerenes C61H2. *Chemical Physics Letters*, **1994**, 228, 490-494	2.5	10
98	A computational evaluation of the water-dimer populations in saturated steam recommended for applications to the Earth, planetary and cometary atmospheres. *Journal of Molecular Structure*, **1992**, 270, 1-9	3.4	10
97	Hydrophobically Modified Amphiphilic Block Copolymer Micelles in Non-Aqueous Polar Solvents. Fluorometric, Light Scattering and Computer-Based Monte Carlo Study. *Collection of Czechoslovak Chemical Communications*, **2002**, 67, 531-556		10
96	Probing the Influence of Phosphine Substituents on the Donor and Catalytic Properties of Phosphinoferrocene Carboxamides: A Combined Experimental and Theoretical Study. *Organometallics*, **2017**, 36, 1828-1841	3.8	9
95	Sc2O@C78: Calculations of the yield ratio for two observed isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2017**, 25, 124-127	1.8	9
94	A fast computational method for determining equilibrium concentration profiles in intermixed nanoislands. *Journal of Physics Condensed Matter*, **2009**, 21, 084217	1.8	9
93	Synthesis and characterisation of Dewar benzene-ferrocene conjugates. *Dalton Transactions*, **2009**, 3137-43	4.3	9
92	Energy–entropy interplay of C60F36 isomers. *Chemical Physics Letters*, **2003**, 374, 100-103	2.5	9
91	Computational studies of atmospheric chemistry species. *Computational and Theoretical Chemistry*, **1993**, 285, 273-276		9

90	Mean squared displacement from fluorescence correlation spectroscopy. *Soft Matter*, **2016**, 12, 3760-9	3.6	9
89	Calculated relative populations for the Eu@C82 isomers. *Chemical Physics Letters*, **2019**, 726, 29-33	2.5	8
88	Stability issues in computational screening of carbon nanostructures: illustrations on La endohedrals. *Molecular Simulation*, **2017**, 43, 1472-1479	2	8
87	Calculated Temperature Development of the Relative Stabilities of Yb@C82 Isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 147-154	1.8	8
86	Fluorescence Spectroscopy as a Tool for Investigating the Self-Organized Polyelectrolyte Systems. *Advances in Polymer Science*, **2010**, 187-249	1.3	8
85	Mg@C74 isomers: Calculated relative concentrations and comparison with Ca@C74. *Physica Status Solidi (A) Applications and Materials Science*, **2007**, 204, 1905-1910	1.6	8
84	A computational thermodynamic evaluation of the altitude profiles of (N2)2, N2-O2 and (O2)2 in the Earth atmosphere. *Thermochimica Acta*, **1994**, 231, 55-60	2.9	8
83	HoO-C: Highly Stretched Cluster Dictated by a Giant Cage and Unexplored Isomerization. *Inorganic Chemistry*, **2020**, 59, 11020-11027	5.1	8
82	Interactions of star-like polyelectrolyte micelles with hydrophobic counterions. *Journal of Colloid and Interface Science*, **2019**, 546, 371-380	9.3	7
81	Towards Relative Populations of Non-Isomeric Metallofullerenes: La@C76( ) vs. La2@C76(,17490). *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 299-306	1.8	7
80	Thermodynamics of small alkali metal halide cluster ions: comparison of classical molecular simulations with experiment and quantum chemistry. *Journal of Physical Chemistry A*, **2015**, 119, 488-500	2.8	7
79	Computational screening of metallofullerenes for nanoscience: Sr@C74. *Molecular Simulation*, **2008** , 34, 17-21	2	7
78	SCF Study of Amphiphilic Micellar Shells Containing Polyelectrolyte and Hydrophobic Sequences. *Macromolecules*, **2007**, 40, 7656-7664	5.5	7
77	Relative Stabilities of C74 Isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2007**, 15, 195-205	1.8	7
76	Isomeric C60F36(g) species: Computed structures and heats of formation. *Physics of the Solid State*, **2002**, 44, 534-535	0.8	7
75	Mean-Field Study of Poly(methacrylic acid) Shells in Partly Hydrophobically Modified Amphiphilic Block Copolymer Micelles in Polar Solvents *Journal of Physical Chemistry B*, **2003**, 107, 8241-8247	3.4	7
74	Thermodynamic Properties of He@C60. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2000**, 8, 453-460		7
73	An estimation of dimerization energetics of the ClO radical. *Chemical Physics Letters*, **1991**, 182, 51-56	2.5	7

72	Multivalent counterions accumulate in star-like polyelectrolytes and collapse the polymer in spite of increasing its ionization. *Soft Matter*, **2020**, 16, 1047-1055	3.6	7
71	Computational Comparison of the Water-Dimer Encapsulations intoD2(22)-C84andD2d(23)-C84. *ECS Journal of Solid State Science and Technology*, **2017**, 6, M3113-M3115	2	6
70	Double-exponential decay of orientational correlations in semiflexible polyelectrolytes. *European Physical Journal E*, **2012**, 35, 53	1.5	6
69	Stimuli-Responsive Amphiphilic Shells of Kinetically Frozen Polymeric Micelles in Aqueous Media: Monte Carlo Simulations and Comparison to Self-Consistent Field Calculations. *Macromolecules*, **2008**, 41, 3711-3719	5.5	6
68	Computations of production yields for Ba@C74 and Yb@C74. *Molecular Simulation*, **2007**, 33, 563-568	2	6
67	AM1 Computations of C60O2. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1994**, 2, 73-88		6
66	Electron Pairing and Chemical Bonds. Physical Meaning of Effective Pairs. *Collection of Czechoslovak Chemical Communications*, **1994**, 59, 2567-2578		6
65	Gas-phase association of O2: a computational thermodynamic study. *Thermochimica Acta*, **1993**, 228, 9-14	2.9	6
64	Computed gas-phase thermodynamics of the N2?O2 complexes. *Thermochimica Acta*, **1993**, 225, 1-7	2.9	6
63	Computational Modeling of the Ce@C82 Metallofullerene Isomeric Composition. *ECS Journal of Solid State Science and Technology*, **2019**, 8, M118-M121	2	6
62	Calculated relative populations of Sm@C82 isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2018**, 26, 233-238	1.8	5
61	Computations on Metallofullerenes Derivatized during Extraction: La@C80-C6H3Cl2 and La@C82-C6H3Cl2. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 173-181	1.8	5
60	Unprecedented chemical reactivity of a paramagnetic endohedral metallofullerene La@C(s)-C82 that leads hydrogen addition in the 1,3-dipolar cycloaddition reaction. *Journal of the American Chemical Society*, **2014**, 136, 17537-46	16.4	5
59	Predicted stabilities of endohedral metallo-fullerenes La@C76. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 2585-2587	1.3	5
58	Synthesis, molecular structure, electrochemistry and DFT study of a ferrocenyl-substituted 4-quinazolinone and related heterocycles. *New Journal of Chemistry*, **2013**, 37, 2019	3.6	5
57	Isolation and Crystallographic Characterization of the Labile Isomer of Y@C82 Cocrystallized with Ni(OEP): Unprecedented Dimerization of Pristine Metallofullerenes. *Angewandte Chemie*, **2016**, 128, 9380-9384	3.6	5
56	Eu@C86 isomers: Calculated relative populations. *Fullerenes Nanotubes and Carbon Nanostructures*, **2020**, 28, 565-570	1.8	4
55	Cyclic water-trimer encapsulation into D2(22)-C84 fullerene. *Chemical Physics Letters*, **2018**, 695, 245-248	2.5	4

54	Depletion profiles for dilute solutions of linear chains, stars and H-branched molecules by self-consistent field calculations and Monte Carlo simulations. *Soft Matter*, **2011**, 7, 10258	3.6	4
53	COMPUTING NARROW NANOTUBES AND THEIR DERIVATIVES. *International Journal of Nanoscience* , **2002**, 01, 303-312	0.6	4
52	The drag of the tails: Diffusion of sticky nanoparticles in dilute polymer solutions. *Journal of Chemical Physics*, **2015**, 143, 243129	3.9	4
51	Calculations of the relative populations of Lu@C82 isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2019**, 27, 710-714	1.8	3
50	Water-Dimer Stability and Its Fullerene Encapsulations. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 2622-2622	0.3	3
49	Sm@C74: Computed Relative Isomeric Populations. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 235-242	1.8	3
48	Monte Carlo simulation of fluorescence correlation spectroscopy data. *Collection of Czechoslovak Chemical Communications*, **2011**, 76, 207-222		3
47	Stability Computations for Fullerenes and Metallofullerenes. *World Scientific Series on Carbon Nanoscience*, **2012**, 381-429	0.5	3
46	Computational Treatment of Alkaline Earth Encapsulations in C74: Relative Thermodynamic Production Abundances. *Fullerenes Nanotubes and Carbon Nanostructures*, **2008**, 16, 507-516	1.8	3
45	Amphiphilic Block Copolymer Micelles with Hydrophobically Modified Shells. *Molecular Simulation*, **2003**, 29, 655-660	2	3
44	Computations of the catalytic effects in the stone□wales fullerene isomerizations: N and CN agents. *International Journal of Quantum Chemistry*, **2004**, 99, 634-639	2.1	3
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42	B3LYP/6-31G*//SAM1 Calculations of C36 Fullerene and quasi-Fullerene Cages. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2000**, 8, 433-447		3
41	AM1 Computed Vibrations in Two C60O Structures. *Spectroscopy Letters*, **1993**, 26, 1785-1796	1.1	3
40	A Computational Study of ClONO2H+: Structure and Vibrations. *Spectroscopy Letters*, **1994**, 27, 563-571	1.1	3
39	A refined evaluation of the gas-phase dimerization thermodynamics of the ClO radical. *International Journal of Thermophysics*, **1992**, 13, 303-313	2.1	3
38	Computed gas-phase thermodynamics of N2 association. *Thermochimica Acta*, **1993**, 223, 1-6	2.9	3
37	Copolymer Micelles with Polyelectrolyte Shell in Aqueous Media. A Mean-Field Study. *Collection of Czechoslovak Chemical Communications*, **2006**, 71, 756-768		3

36	Rotameric Isomers of La2@C80 & Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization. *ECS Journal of Solid State Science and Technology*, **2020**, 9, 061014	2	3
35	Calculations of the Lu3N@C80 two-isomer equilibrium. *Fullerenes Nanotubes and Carbon Nanostructures*, **2019**, 27, 382-386	1.8	3
34	An analytical solution of isotopomeric enumerations for C2v cyclic odd-numbered carbon clusters Cn. *Journal of Radioanalytical and Nuclear Chemistry*, **1997**, 219, 69-71	1.5	2
33	Computations of endohedral fullerenes: The Gibbs energy treatment. *Journal of Computational Methods in Sciences and Engineering*, **2006**, 6, 243-250	0.3	2
32	Two Isomers of C60F48: Computed Inter-isomeric Equilibrium. *Fullerenes Nanotubes and Carbon Nanostructures*, **2003**, 11, 219-226	1.8	2
31	Computations of Low-Energy Non-Icosahedral Structures of C60. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2000**, 8, 403-415		2
30	Metal-Coated Fullerenes C60Mn: Calculations for M = Be, Mg, Al AND n = 12, 20, 32. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2000**, 8, 385-402		2
29	C61H2 Fulleroid: AM1 Computational Study. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1994**, 2, 13-24		2
28	A computational evaluation of the ozone dimer altitude profile. *Thermochimica Acta*, **1994**, 232, 1-6	2.9	2
27	A computational evaluation of relative stabilities of the open C2v and cyclic D3h forms of ozone. *Thermochimica Acta*, **1992**, 196, 459-465	2.9	2
26	Calculations on endohedral C74 complexes. *Journal of Nanoscience and Nanotechnology*, **2007**, 7, 1339-45	1.3	2
25	Intramolecular micellization and nanopatterning in pH- and thermo-responsive molecular brushes. *Soft Matter*, **2020**, 16, 208-218	3.6	2
24	Calculated relative populations for the Eu@C84 isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2021**, 29, 144-148	1.8	2
23	Quantum-chemical calculations of the metallofullerene yields in the X@C74, L@C74, and Z@C82 series **2015**,		1
22	Predicting stabilities of endohedral metallofullerenes Yb@C84. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 2709-2712	1.3	1
21	Carbon Nanostructures: Calculations of their Energetics, Thermodynamics, and Stability491-523		1
20	Computations of the Energetics of C60F36 Isomers. *Fullerenes Nanotubes and Carbon Nanostructures*, **2006**, 14, 57-65	1.8	1
19	A computational study of entropy rules for charged fullerenes. *Physics of the Solid State*, **2002**, 44, 548-550	1.8	1

18	A MODEL STUDY OF NARROW NANOTUBES RELATED TO C36, C32, C20, AND C16: SEMIEMPIRICAL AND NONEMPIRICAL TREATMENTS. *Fullerenes Nanotubes and Carbon Nanostructures*, **2002**, 10, 207-215	1.8	1
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