Manuel Alcami

List of Publications by Year
in descending order

187	5,079	94433	118850
papers	citations	37 h-index	62 g-index

194	194	194	5216
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Controlling the diversity of ion-induced fragmentation pathways by N-methylation of amino acids. Physical Chemistry Chemical Physics, 2022, 24, 941-954.	2.8	3
2	A general approach to study molecular fragmentation and energy redistribution after an ionizing event. Physical Chemistry Chemical Physics, 2021, 23, 1859-1867.	2.8	9
3	Charge and energy sharing in the fragmentation of astrophysically relevant carbon clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	1
4	Roadmap on dynamics of molecules and clusters in the gas phase. European Physical Journal D, 2021, 75, 1.	1.3	32
5	Hydrogenation of C₂₄ Carbon Clusters: Structural Diversity and Energetic Properties. Journal of Physical Chemistry A, 2021, 125, 5273-5288.	2.5	5
6	Timing of charge migration in betaine by impact of fast atomic ions. Science Advances, 2021, 7, eabg9080.	10.3	2
7	Understanding the formation of metastable furan dication in collisions with ions. Journal of Physics: Conference Series, 2020, 1412, 132002.	0.4	0
8	Polypeptide formation in clusters of Î²-alanine amino acids by single ion impact. Nature Communications, 2020, 11, 3818.	12.8	22
9	Hydrogenated polycyclic aromatic hydrocarbons: isomerism and aromaticity. Physical Chemistry Chemical Physics, 2020, 22, 21968-21976.	2.8	7
10	When is the Bellâ€“Evansâ€“Polanyi principle fulfilled in Dielsâ€“Alder reactions of fullerenes?. Physical Chemistry Chemical Physics, 2020, 22, 8846-8852.	2.8	5
11	Foreword to the special issue on the â€œElectronic structure: principles and applications (ESPA 2018)â€• conference. Theoretical Chemistry Accounts, 2020, 139, 86.	1.4	0
12	Isomers of Hydrogenated Polycyclic Aromatic Hydrocarbons Explain the Presence of Infrared Bands in the 3 Î¼m Region. Astrophysical Journal, 2020, 899, 18.	4.5	5
13	Determination of energy-transfer distributions in ionizing ion-molecule collisions. Journal of Physics: Conference Series, 2020, 1412, 152085.	0.4	0
14	Decay pathways for protonated and deprotonated adenine molecules. Journal of Chemical Physics, 2019, 151, 044306.	3.0	0
15	Fully versus constrained statistical fragmentation of carbon clusters and their heteronuclear derivatives. Journal of Chemical Physics, 2019, 150, 144301.	3.0	4
16	Theoretical Study of NO Dissociation on an Open Flat Ru(101Ì…1) Surface. Journal of Physical Chemistry C, 2019, 123, 5488-5494.	3.1	0
17	Aromaticity, Coulomb repulsion, Ï€ delocalization or strain: who is who in endohedral metallofullerene stability?. Physical Chemistry Chemical Physics, 2019, 21, 124-131.	2.8	7
18	Simple bond patterns predict the stability of Dielsâ€“Alder adducts of empty fullerenes. Chemical Communications, 2018, 54, 4156-4159.	4.1	10

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19	Topology-Based Approach to Predict Relative Stabilities of Charged and Functionalized Fullerenes. Journal of Chemical Theory and Computation, 2018, 14, 1791-1810.	5.3	21
20	Furan Fragmentation in the Gas Phase: New Insights from Statistical and Molecular Dynamics Calculations. Journal of Physical Chemistry A, 2018, 122, 4153-4166.	2.5	19
21	Computational Study of the Structure and Degradation Products of Alloxydim Herbicide. Journal of Physical Chemistry A, 2018, 122, 3909-3918.	2.5	7
22	Pesticide byproducts formation: Theoretical study of the protonation of alloxydim degradation products. Computational and Theoretical Chemistry, 2018, 1143, 9-19.	2.5	8
23	Tribute to Manuel YÃ¡Ã±ez and Otilia MÃ³. Journal of Physical Chemistry A, 2018, 122, 5671-5672.	2.5	0
24	Relative Stability of Empty Exohedral Fullerenes: Ï€ Delocalization versus Strain and Steric Hindrance. Journal of the American Chemical Society, 2017, 139, 1609-1617.	13.7	36
25	Generalized structural motif model for studying the thermodynamic stability of fullerenes: from C₆₀to graphene passing through giant fullerenes. Physical Chemistry Chemical Physics, 2017, 19, 19646-19655.	2.8	9
26	Quantum chemistry in environmental pesticide risk assessment. Pest Management Science, 2017, 73, 2199-2202.	3.4	21
27	Production of doubly-charged highly reactive species from the long-chain amino acid GABA initiated by Ar⁹⁺ionization. Physical Chemistry Chemical Physics, 2017, 19, 19609-19618.	2.8	13
28	M₃C: A Computational Approach To Describe Statistical Fragmentation of Excited Molecules and Clusters. Journal of Chemical Theory and Computation, 2017, 13, 992-1009.	5.3	20
29	Tuning Intermolecular Charge Transfer in Donorâ€“Acceptor Two-Dimensional Crystals on Metal Surfaces. Journal of Physical Chemistry C, 2017, 121, 23505-23510.	3.1	11
30	XUV/X-ray light and fast ions for ultrafast chemistry. Physical Chemistry Chemical Physics, 2017, 19, 19533-19535.	2.8	0
31	Charge dependence of fragmentation process induced by ion collisions with furan molecule. Journal of Physics: Conference Series, 2017, 875, 102021.	0.4	1
32	Excitation and fragmentation in high velocity C_nN⁺- He collisions. Journal of Physics: Conference Series, 2017, 875, 102022.	0.4	1
33	Mechanical Isolation of Highly Stable Antimonene under Ambient Conditions. Advanced Materials, 2016, 28, 6332-6336.	21.0	444
34	Fragmentation network of doubly charged methionine: Interpretation using graph theory. Journal of Chemical Physics, 2016, 145, 094302.	3.0	3
35	Understanding the self-assembly of TCNQ on Cu(111): a combined study based on scanning tunnelling microscopy experiments and density functional theory simulations. RSC Advances, 2016, 6, 15071-15079.	3.6	22
36	Adsorption of Hydrogen Molecules on Carbon Nanotubes Using Quantum Chemistry and Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 6451-6458.	2.5	45

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37	Antimonene: Mechanical Isolation of Highly Stable Antimonene under Ambient Conditions (Adv. Mater.) Tj ETQq1 1 0.784314 rgBT /Ove	21.0	23
38	Determination of Energy-Transfer Distributions in Ionizing Ion-Molecule Collisions. Physical Review Letters, 2016, 117, 073201.	7.8	39
39	Atomically resolved phase transition of fullerene cations solvated in helium droplets. Nature Communications, 2016, 7, 13550.	12.8	84
40	Thermal Transition from a Disordered, 2D Network to a Regular, 1D, Fe(II)â€“DCNQI Coordination Network. Journal of Physical Chemistry C, 2016, 120, 16712-16721.	3.1	4
41	Theoretical study of the interaction between molecular hydrogen and [MC₆₀]⁺ complexes. RSC Advances, 2016, 6, 27447-27451.	3.6	7
42	Key Structural Motifs To Predict the Cage Topology in Endohedral Metallofullerenes. Journal of the American Chemical Society, 2016, 138, 1551-1560.	13.7	36
43	Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C_nH_m^{q+} (n = 1â€“5, m =) Tj ETQq1 1 0.784314 rgB	2.8	28
44	Is C50 a superaromat? Evidence from electronic structure and ring current calculations. Physical Chemistry Chemical Physics, 2016, 18, 11653-11660.	2.8	12
45	Structure, Ionization and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: C_nH^{q+}_m (n = 1 â” 5, m =) Tj ETQq1 1 0.784314 rgB	2.8	28
46	Surfaceâ€Supported Robust 2D Lanthanideâ€Carboxylate Coordination Networks. Small, 2015, 11, 6358-6364.	10.0	43
47	Molecular dynamics of photodissociation: towards more complex systems. Journal of Physics: Conference Series, 2015, 635, 112105.	0.4	1
48	Breakdown curves of carbon-based molecules for astrochemistry. Journal of Physics: Conference Series, 2015, 635, 032107.	0.4	0
49	Theoretical Modeling of Mass Spectrometry. Journal of Physics: Conference Series, 2015, 635, 072060.	0.4	0
50	X-ray induced fragmentation dynamics of doubly charged L-alanine in gas phase. Journal of Physics: Conference Series, 2015, 635, 112094.	0.4	1
51	Slow ion interaction with N-methylglycine and N-acetylglycine. Journal of Physics: Conference Series, 2015, 635, 032054.	0.4	0
52	Molecular dynamics studies of impulse driven reactions in molecules and molecular clusters. Journal of Physics: Conference Series, 2015, 635, 032043.	0.4	1
53	Unusual hydrogen and hydroxyl migration in the fragmentation of excited doubly-positively-charged amino acids in the gas phase. Journal of Physics: Conference Series, 2015, 635, 032037.	0.4	0
54	Fusion reaction dynamics of fullerene molecules. Journal of Physics: Conference Series, 2015, 635, 032093.	0.4	0

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55	Unusual hydroxyl migration in the fragmentation of Î²-alanine dication in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 16767-16778.	2.8	29
56	Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Moleculeâ€“Substrate Interaction and Decoupling. Journal of Physical Chemistry C, 2015, 119, 4062-4071.	3.1	20
57	Internal energy dependence in x-ray-induced molecular fragmentation: An experimental and theoretical study of thiophene. Physical Review A, 2015, 91, .	2.5	36
58	Molecular Growth Inside of Polycyclic Aromatic Hydrocarbon Clusters Induced by Ion Collisions. Journal of Physical Chemistry Letters, 2015, 6, 1536-1542.	4.6	62
59	Cage connectivity and frontier Ï€ orbitals govern the relative stability of charged fullerene isomers. Nature Chemistry, 2015, 7, 927-934.	13.6	41
60	N-Acetylglycine Cation Tautomerization Enabled by the Peptide Bond. Journal of Physical Chemistry A, 2015, 119, 9581-9589.	2.5	5
61	Bonding in exohedral metalâ€“fullerene cationic complexes. RSC Advances, 2014, 4, 53010-53020.	3.6	18
62	Multiple ionization and hydrogen loss from neutral and positively-charged coronene. Journal of Chemical Physics, 2014, 140, 204307.	3.0	31
63	Ultrafast nonadiabatic fragmentation dynamics of biomolecules. Journal of Physics: Conference Series, 2014, 488, 012037.	0.4	7
64	Time-dependent density functional theory molecular dynamics simulation of doubly charged uracil in gas phase. Open Physics, 2014, 12, .	1.7	4
65	Charge transfer-assisted self-limited decyanation reaction of TCNQ-type electron acceptors on Cu(100). Chemical Communications, 2014, 50, 833-835.	4.1	16
66	Charge-Transfer-Induced Isomerization of DCNQI on Cu(100). Journal of Physical Chemistry C, 2014, 118, 27388-27392.	3.1	3
67	Controlling the spatial arrangement of organic magnetic anions adsorbed on epitaxial graphene on Ru(0001). Nanoscale, 2014, 6, 15271-15279.	5.6	19
68	Multiple electron capture, excitation, and fragmentation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:msup><mml:mrow /><mml:mrow><mml:mn>6</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup><mml:mo>â^’</mml:mo></mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>collisions. Physical Review A, 2014, 90, .	2.5	8
69	Probing the Site-Dependent Kondo Response of Nanostructured Graphene with Organic Molecules. Nano Letters, 2014, 14, 4560-4567.	9.1	24
70	Stability of the glycine cation in the gas phase after interaction with multiply charged ions. European Physical Journal D, 2014, 68, 1.	1.3	16
71	Unraveling the Factors That Control Soft Landing of Small Silyl Ions on Fluorinated Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 10159-10169.	3.1	5
72	Chain-Length and Temperature Dependence of Self-Assembled Monolayers of Alkylthiolates on Au(111) and Ag(111) Surfaces. Journal of Physical Chemistry A, 2014, 118, 4138-4146.	2.5	23

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73	Non-statistical fragmentation of PAHs and fullerenes in collisions with atoms. International Journal of Mass Spectrometry, 2014, 365-366, 260-265.	1.5	34
74	Fragmentation Dynamics of Doubly Charged Methionine in the Gas Phase. Journal of Physical Chemistry A, 2014, 118, 1374-1383.	2.5	22
75	Formation dynamics of fullerene dimers<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi>C</mml:mi><mml:mrow><mml:mn>118</mml:mn><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mrow></mml:msubsup></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi>C</mml:mi><mml:mrow><mml:mn>119</mml:mn><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mrow></mml:msubsup></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msubsup><mml:mi>C</mml:mi><mml:mrow><mml:mn>120</mml:mn><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:mrow></mml:msubsup></mml:math>. Physical Review A, 2014, 89, .	2.5	27
76	Fragmentation of amino acids induced by collisions with low-energy highly charged ions. Journal of Physics: Conference Series, 2014, 488, 102019.	0.4	0
77	Bond formation in C+59 â€“ C60 collisions. Journal of Physics: Conference Series, 2014, 488, 012028.	0.4	0
78	Fragmentation dynamics of excited ionized polycyclic aromatic hydrocarbons. Journal of Physics: Conference Series, 2014, 488, 102027.	0.4	0
79	Exohedral interaction in cationic lithium metallofullerenes. Highlights in Theoretical Chemistry, 2014, , 89-96.	0.0	0
80	Exohedral interaction in cationic lithium metallofullerenes. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	7
81	Onset of Chiral Adenine Surface Growth. ChemPhysChem, 2013, 14, 3294-3302.	2.1	2
82	Ultrafast Damage Following Radiationâ€Induced Oxidation of Uracil in Aqueous Solution. Angewandte Chemie - International Edition, 2013, 52, 3160-3163.	13.8	34
83	Dynamics of Glycine Dications in the Gas Phase: Ultrafast Intramolecular Hydrogen Migration versus Coulomb Repulsion. Journal of Physical Chemistry Letters, 2013, 4, 3903-3909.	4.6	74
84	Lattice-matched versus lattice-mismatched models to describe epitaxial monolayer graphene on Ru(0001). Physical Review B, 2013, 88, .	3.2	35
85	Density functional theory study of the structure and vibrational modes of acrylonitrile adsorbed on Cu(100). Physical Chemistry Chemical Physics, 2013, 15, 1288-1295.	2.8	11
86	Elastic Response of Graphene Nanodomes. ACS Nano, 2013, 7, 2927-2934.	14.6	35
87	Long-range magnetic order in a purely organic 2D layer adsorbed on epitaxial graphene. Nature Physics, 2013, 9, 368-374.	16.7	158
88	Ordered arrays of metalâ€“organic magnets at surfaces. Journal of Physics Condensed Matter, 2013, 25, 484007.	1.8	16
89	Ions colliding with clusters of fullerenesâ€”Decay pathways and covalent bond formations. Journal of Chemical Physics, 2013, 139, 034309.	3.0	21
90	Formations of Dumbbell<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>118</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">C</mml:mi><mml:mn>119</mml:mn></mml:msub></mml:math>inside Clusters of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:m	7.8	61

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91	Electron localization in epitaxial graphene on Ru(0001) determined by moirÃ© corrugation. Physical Review B, 2012, 85, .	3.2	34
92	Charge transfer and fragmentation in C60+ C6+collisions. Journal of Physics: Conference Series, 2012, 388, 102012.	0.4	0
93	Commensurate Solidâ€“Solid Phase Transitions in Self-Assembled Monolayers of Alkylthiolates Lying on Metal Surfaces. Journal of the American Chemical Society, 2012, 134, 13224-13227.	13.7	11
94	Ultrafast non-adiabatic fragmentation dynamics of doubly charged uracil in gas and liquid phase. Journal of Physics: Conference Series, 2012, 388, 102055.	0.4	1
95	Structures, Energetics, and Dynamics of Helium Adsorbed on Isolated Fullerene Ions. Physical Review Letters, 2012, 108, 076101.	7.8	68
96	A Multicoincidence Study of Fragmentation Dynamics in Collision of Î³â€Aminobutyric Acid with Lowâ€Energy Ions. Chemistry - A European Journal, 2012, 18, 9321-9332.	3.3	44
97	Theoretical study of the structure of self-assembled monolayers of short alkylthiolates on Au(111) and Ag(111): the role of induced substrate reconstruction and chainâ€“chain interactions. Physical Chemistry Chemical Physics, 2011, 13, 9353.	2.8	24
98	Formation of Self-Assembled Chains of Tetrathiafulvalene on a Cu(100) Surface. Journal of Physical Chemistry A, 2011, 115, 13080-13087.	2.5	6
99	Surface assembly of porphyrin nanorods with one-dimensional zincâ€“oxygen spinal cords. CrystEngComm, 2011, 13, 5591.	2.6	8
100	A density functional theory study of the manganese-phthalocyanine. Theoretical Chemistry Accounts, 2011, 128, 497-503.	1.4	30
101	Theoretical study of the stability of small triply charged carbon clusters Cn3+ (n=3â€“12). International Journal of Mass Spectrometry, 2011, 299, 20-26.	1.5	2
102	Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase. Physical Review Letters, 2011, 107, 023202.	7.8	63
103	Role of Dispersion Forces in the Structure of Graphene Monolayers on Ru Surfaces. Physical Review Letters, 2011, 106, 186102.	7.8	129
104	Charge-transfer-induced structural rearrangements at both sides of organic/metal interfaces. Nature Chemistry, 2010, 2, 374-379.	13.6	273
105	Magic and hot giant fullerenes formed inside ion irradiated weakly bound C60 clusters. Journal of Chemical Physics, 2010, 133, 104301.	3.0	28
106	Growth and Structure of Self-assembled Monolayers of a TTF Derivative on Au(111). Journal of Physical Chemistry C, 2010, 114, 6503-6510.	3.1	16
107	Theoretical investigation of the ultrafast dissociation of ionised biomolecules immersed in water: Direct and indirect effects. Mutation Research - Reviews in Mutation Research, 2010, 704, 45-53.	5.5	31
108	Study of the interaction between short alkanethiols from ab initio calculations. Physical Chemistry Chemical Physics, 2010, 12, 7555.	2.8	17

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109	Density functional theory study of multiply ionized weakly bound fullerene dimers. Journal of Chemical Physics, 2009, 130, 224302.	3.0	14
110	Ionization and fragmentation of water clusters by fast highly charged ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 075101.	1.5	22
111	Stability of multiply charged fullerene anions and cations. Physical Review A, 2009, 80, .	2.5	11
112	Absolute charge transfer and fragmentation cross sections in He2++C60collisions. Journal of Physics: Conference Series, 2009, 194, 012047.	0.4	2
113	Stable Nonâ€IPR C₆₀ and C₇₀ Fullerenes Containing a Uniform Distribution of Pyrenes and Adjacent Pentagons. ChemPhysChem, 2008, 9, 861-866.	2.1	39
114	Understanding the Supramolecular Selfâ€Assembly of the Fullerene Derivative PCBM on Gold Surfaces. ChemPhysChem, 2008, 9, 1030-1035.	2.1	21
115	Absolute Charge Transfer and Fragmentation Cross Sections inHe2+â^'C60Collisions. Physical Review Letters, 2008, 100, 183401.	7.8	31
116	Theoretical study of the stability of multiply charged C70 fullerenes. Journal of Chemical Physics, 2007, 127, 104308.	3.0	16
117	First- and second-electron affinities ofC60andC70isomers. Physical Review A, 2007, 76, .	2.5	30
118	Structural Patterns in Fullerenes Showing Adjacent Pentagons: C20 to C72. Journal of Nanoscience and Nanotechnology, 2007, 7, 1329-1338.	0.9	26
119	Crossover Siteâ€Selectivity in the Adsorption of the Fullerene Derivative PCBM on Au(111). Angewandte Chemie - International Edition, 2007, 46, 7874-7877.	13.8	70
120	Unimolecular Reactivity of Uracilâ€“Cu2+ Complexes in the Gas Phase. ChemPhysChem, 2007, 8, 181-187.	2.1	64
121	Gas-Phase Deprotonation of Uracilâ^'Cu2+ and Thiouracilâ^'Cu2+ Complexes. Journal of Physical Chemistry A, 2006, 110, 1943-1950.	2.5	69
122	Structure of <mml:math altimg="si1.gif" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsevier.com/x	3.0	6
123	Ionization potentials, dissociation energies and statistical fragmentation of neutral and positively charged small carbon clusters. Brazilian Journal of Physics, 2006, 36, 529-533.	1.4	20
124	Ionization potentials and dissociation energies of neutral, singly and doubly charged Cn fullerenes from n=20 to 70. International Journal of Mass Spectrometry, 2006, 252, 133-141.	1.5	29
125	Fragmentation of small neutral carbon clusters. International Journal of Mass Spectrometry, 2006, 252, 126-132.	1.5	21
126	Understanding Sulfone Behavior in Palladium-Catalyzed Domino Reactions with Aryl Iodides. Chemistry - A European Journal, 2006, 12, 4576-4583.	3.3	18

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127	Computational Studies on the Cyclization of Polycyclic Aromatic Hydrocarbons in the Synthesis of Curved Aromatic Derivatives. ChemPhysChem, 2006, 7, 475-481.	2.1	3
128	FRAGMENTATION OF COLLISIONALLY EXCITED FULLERENES. , 2006, , .		0
129	Fullerene C50: Sphericity takes over, not strain. Chemical Physics Letters, 2005, 407, 153-158.	2.6	56
130	Size dependence of ionization potentials and dissociation energies for neutral and singly-charged Cn fullerenes (n=40â€“70). Chemical Physics Letters, 2005, 416, 14-17.	2.6	22
131	Coulomb Stability Limit of Highly ChargedC60q+Fullerenes. Physical Review Letters, 2005, 95, 013401.	7.8	55
132	Structure and Electronic Properties of Fullerenes C52q+: Is C522+an Exception to the Pentagon Adjacency Penalty Rule?. ChemPhysChem, 2005, 6, 92-100.	2.1	43
133	Why Does Pivalaldehyde (Trimethylacetaldehyde) Unexpectedly Seem More Basic Than 1-Adamantanecarbaldehyde in the Gas Phase? FT-ICR and High-Level Ab Initio Studies. Chemistry - A European Journal, 2005, 11, 1826-1832.	3.3	13
134	Statistical fragmentation of small neutral carbon clusters. Physical Review A, 2005, 71, .	2.5	34
135	Structure and electronic properties of highly charged C60 and C58 fullerenes. Journal of Chemical Physics, 2005, 123, 184306.	3.0	41
136	Structure and reactivity of C54q+(q= 0, 1, 2 and 4) fullerenes. Physical Chemistry Chemical Physics, 2005, 7, 3756.	2.8	4
137	Optimization of extended basis sets and assessment of different theoretical schemes for Pb containing compounds. Chemical Physics Letters, 2004, 383, 561-565.	2.6	14
138	Association of Cu2+with Uracil and Its Thio Derivatives: A Theoretical Study. ChemPhysChem, 2004, 5, 1871-1878.	2.1	66
139	Unimolecular Reactivity of Strong Metalâ€“Cation Complexes in the Gas Phase: Ethylenediamineâ€“Cu+. Chemistry - A European Journal, 2004, 10, 2927-2934.	3.3	24
140	Theoretical Survey of the Potential Energy Surface of Ethylenediamine + Cu+Reactions. Journal of Physical Chemistry A, 2004, 108, 8367-8372.	2.5	22
141	Fragmentation of Highly Excited Small Neutral Carbon Clusters. Physical Review Letters, 2004, 93, 063401.	7.8	45
142	Charge Transfer and Evaporation in Low Energy Collisions of Metal Clusters and Fullerenes with Atomic Targets. Physica Scripta, 2004, 110, 308.	2.5	2
143	Fragmentation of neutral Cn clusters (n ? 9): experimental and theoretical investigations. European Physical Journal D, 2003, 24, 149-152.	1.3	8
144	Gas-Phase Reactivity of Uracil, 2-Thiouracil, 4-Thiouracil, and 2,4-Dithiouracil towards the Cu+ Cation: A DFT Study. ChemPhysChem, 2003, 4, 1011-1016.	2.1	45

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145	Gas-Phase Chemistry of Ethynylamine, -Phosphine and -Arsine. Structure and Stability of their Cu+ and Ni+ Complexes. ChemPhysChem, 2003, 4, 72-78.	2.1	5
146	The Final Steps of the Oppolzer Cyclization: Mechanism of the Insertion of Alkenes into Allylpalladium(II) Complexes. Chemistry - A European Journal, 2003, 9, 96-105.	3.3	19
147	Theoretical study of ionization potentials and dissociation energies of Cnq+ fullerenes (n=50â€“60,) Tj ETQq1 1 0.784314 rgBT /Over	3.0	78
148	Structure, Dissociation Energies, and Harmonic Frequencies of Small Doubly Charged Carbon Clusters Cn2+(n= 3â˜9)â€. Journal of Physical Chemistry A, 2002, 106, 10782-10789.	2.5	31
149	Gas-Phase Basicity of 2,7-Dimethyl-[1,2,4]-Triazepine Thio Derivatives. Journal of Physical Chemistry A, 2002, 106, 7383-7389.	2.5	18
150	Experimental and Theoretical Investigation of the Reactions between Glucose and Cu+ in the Gas Phase. Journal of Physical Chemistry A, 2002, 106, 2641-2651.	2.5	28
151	Prototropic tautomerism of 3,5-(oxo/thioxo) derivatives of 2,7-dimethyl-1,2,4-triazepinesElectronic supplementary information (ESI) available: the B3LYP/6-31G* optimized geometries of all the structures included in Fig. 1 and the corresponding TS. See http://www.rsc.org/suppdata/nj/b1/b109397e/. New Journal of Chemistry, 2002, 26, 711-719.	2.8	13
152	Gas-Phase Chemistry of Ethyl and Vinyl Amines, Phosphines, and Arsines:â€‰ A DFT Study of the Structure and Stability of Their Cu+ Complexes. Journal of Physical Chemistry A, 2002, 106, 9306-9312.	2.5	10
153	Triaziridine and tetrazetidine vs. cyclic water trimer and tetramer: A computational approach to the relationship between molecular and supramolecular conformational analysis. Physical Chemistry Chemical Physics, 2002, 4, 2123-2129.	2.8	10
154	A theoretical study of the interaction between Ni+ and small oxygen- and nitrogen-containing bases. International Journal of Mass Spectrometry, 2002, 217, 119-129.	1.5	16
155	Modeling intrinsic basicities and acidities. Journal of Physical Organic Chemistry, 2002, 15, 174-186.	1.9	57
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