Stefano Borocci

List of Publications by Year in descending order

82 papers	1,299 citations	304602 22 h-index	414303 32 g-index
86 all docs	86 docs citations	86 times ranked	1196 citing authors

#	Article	IF	Citations
1	Noble-gas compounds: A general procedure of bonding analysis. Journal of Chemical Physics, 2022, 156, 014104.	1.2	10
2	Design and Characterization of Myristoylated and Non-Myristoylated Peptides Effective against Candida spp. Clinical Isolates. International Journal of Molecular Sciences, 2022, 23, 2164.	1.8	10
3	On the Proton-Bound Noble Gas Dimers (Ng-H-Ng)+ and (Ng-H-Ngâ€™)+ (Ng, Ngâ€™ = He-Xe): Relationships between Structure, Stability, and Bonding Character. Molecules, 2021, 26, 1305.	1.7	8
4	From LAr to L-ArBeO (LÂ=ÂHe, Ne, Ar, HF): Switching on Ïƒ-hole effects in non-covalent interactions. Chemical Physics Letters, 2021, 768, 138402.	1.2	8
5	Altered Local Interactions and Long-Range Communications in UK Variant (B.1.1.7) Spike Glycoprotein. International Journal of Molecular Sciences, 2021, 22, 5464.	1.8	9
6	Concerning the Role of Ïƒ-Hole in Non-Covalent Interactions: Insights from the Study of the Complexes of ArBeO with Simple Ligands. Molecules, 2021, 26, 4477.	1.7	2
7	Ionization of 2â€•and 4(5)â€Nitroimidazoles Radiosensitizers: A â€œKinetic Competitionâ€ Between NO₂ and NO Losses. ChemPhysChem, 2021, 22, 2387-2391.	1.0	5
8	How stereochemistry of lipid components can affect lipid organization and the route of liposome internalization into cells. Nanoscale, 2021, 13, 11976-11993.	2.8	8
9	Multiple Recombination Events and Strong Purifying Selection at the Origin of SARS-CoV-2 Spike Glycoprotein Increased Correlated Dynamic Movements. International Journal of Molecular Sciences, 2021, 22, 80.	1.8	21
10	VUV Photofragmentation of Chloroiodomethane: The Iso-CH2Iâ€“Cl and Iso-CH2Clâ€“I Radical Cation Formation. Journal of Physical Chemistry A, 2020, 124, 7491-7499.	1.1	5
11	Classifying the chemical bonds involving the noble-gas atoms. New Journal of Chemistry, 2020, 44, 14536-14550.	1.4	17
12	Complexes of helium with neutral molecules: Progress toward a quantitative scale of bonding character. Journal of Computational Chemistry, 2020, 41, 1000-1011.	1.5	10
13	Complexes of the noble-gas atoms with unsaturated ions: A theoretical investigation on the exemplary (H2CÂ=ÂNH2+)Ar. Chemical Physics Letters, 2020, 752, 137532.	1.2	1
14	Noncovalent Complexes of the Nobleâ€Gas Atoms: Analyzing the Transition from Physical to Chemical Interactions. Journal of Computational Chemistry, 2019, 40, 2318-2328.	1.5	19
15	Complexation of short ds RNA/DNA oligonucleotides with Gemini micelles: a time resolved SAXS and computational study. Physical Chemistry Chemical Physics, 2017, 19, 3046-3055.	1.3	6
16	â€œPositionâ€•does matter : the photofragmentation of the nitroimidazole isomers. Journal of Physics: Conference Series, 2017, 875, 032007.	0.3	0
17	Communication: â€œPositionâ€•does matter: The photofragmentation of the nitroimidazole isomers. Journal of Chemical Physics, 2016, 145, 191102.	1.2	25
18	Complexes of the Noble Gases with H3O+: A Theoretical Investigation of Ng(H3O+) (Ng = Heâ€”Xe). European Journal of Mass Spectrometry, 2015, 21, 171-181.	0.5	7

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19	Bimolecular Homolytic Substitutions at Nitrogen: An Experimental and Theoretical Study on the Gasâ€Phase Reactions of Alkyl Radicals with NF₃. Chemistry - A European Journal, 2015, 21, 15826-15834.	1.7	5
20	New insight on the photofragmentation of CH₂I₂. Journal of Physics: Conference Series, 2015, 635, 112064.	0.3	0
21	Bonding Motifs of Noble-Gas Compounds As Described by the Local Electron Energy Density. Journal of Physical Chemistry A, 2015, 119, 6528-6541.	1.1	42
22	VUV Photofragmentation of CH₂I₂: The [CH₂Iâ€“I]^{â€¢+} Iso-diiodomethane Intermediate in the I-Loss Channel from [CH₂I₂]^{â€¢+}. Journal of Physical Chemistry A, 2015, 119, 3704-3709.	1.1	12
23	Role of the hydrophilic spacer of glucosylated amphiphiles included in liposome formulations in the recognition of Concanavalin A. Colloids and Surfaces B: Biointerfaces, 2015, 136, 232-239.	2.5	11
24	Complexes of XeHXe⁺ with Simple Ligands: A Theoretical Investigation on (XeHXe⁺)L (L = N₂, CO, H₂O, NH₃). Journal of Physical Chemistry A, 2015, 119, 2383-2392.	1.1	22
25	Isomerism of Cycloserine and Its Protonated Form. ChemPlusChem, 2014, 79, 584-591.	1.3	5
26	Neutral Compounds with Xenonâ€“Germanium Bonds: A Theoretical Investigation on FXeGeF and FXeGeF3. Journal of Physical Chemistry A, 2014, 118, 3326-3334.	1.1	21
27	Recognition of Concanavalin A by Cationic Glucosylated Liposomes. Langmuir, 2014, 30, 11301-11306.	1.6	23
28	Ion chemistry of sulfuryl fluoride: An experimental and theoretical study on gas-phase reactions involving neutral and ionized SO2F2. International Journal of Mass Spectrometry, 2013, 354-355, 46-53.	0.7	0
29	Synthesis and physicochemical characterization of pyrrolidinium based surfactants. Journal of Colloid and Interface Science, 2013, 392, 297-303.	5.0	12
30	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:msup><mml:mrow><mml:mtext>HNg</mml:mtext></mml:mrow><mml:mrow><mml:mo>+</mml:m stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mtext>OH</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m	1.1	5
31	Germyl Cations with Geâ€“S Bonds: An Experimental and Theoretical Study on the Gaseous F_nGe(SH)⁺_{3â€“n} (n = 0â€“2). European Journal of Mass Spectrometry, 2012, 18, 447-456.	0.5	1
32	Gaseous germyl cations: A theoretical investigation on the structure, properties, and mechanism of formation of and (n=0â€“2). Computational and Theoretical Chemistry, 2012, 993, 131-139.	1.1	6
33	Gasâ€phase reactions of SiH_n⁺ (n = 1,2) with NF₃: A computational investigation on the detailed mechanistic aspects. Journal of Computational Chemistry, 2012, 33, 1918-1926.	1.5	3
34	New pyrenyl fluorescent amphiphiles: synthesis and aggregation properties. Soft Matter, 2011, 7, 8525.	1.2	8
35	Segregation into domains observed in liquid crystal phases: comparison of experimental and theoretical data. Soft Matter, 2011, 7, 3392.	1.2	3
36	Positive Ion Chemistry of SiH₄/GeF₄ Gaseous Mixtures Studied by Ion Trap Mass Spectrometry and Ab Initio Calculations. European Journal of Mass Spectrometry, 2011, 17, 197-206.	0.5	2

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37	Gasâ€phase chemistry of ionized and protonated GeF₄: a joint experimental and theoretical study. Journal of Mass Spectrometry, 2011, 46, 465-477.	0.7	10
38	Xenonâ€“Nitrogen Chemistry: Gasâ€Phase Generation and Theoretical Investigation of the Xenonâ€“Difluoronitrenium Ion F₂Nï£¿Xe⁺. Chemistry - A European Journal, 2011, 17, 10682-10689.	1.7	40
39	Cationic noble gas hydrides-2: A theoretical investigation on HNgHNgH+ (Ng=Ar, Kr, Xe). Computational and Theoretical Chemistry, 2011, 964, 318-323.	1.1	19
40	F3Geâ^'Xe+: A Xenonâ^'Germanium Molecular Species. Journal of Physical Chemistry Letters, 2010, 1, 2006-2010.	2.1	39
41	Cationic Noble Gas Hydrides: A Theoretical Investigation of Dinuclear HNgFNgH⁺(Ng =) Tj ETQq1 1 0.784314 rgBT /Over	1.1	29
42	Efficiency of Liposomes in the Delivery of a Photosensitizer Controlled by the Stereochemistry of a Gemini Surfactant Component. Molecular Pharmaceutics, 2010, 7, 130-137.	2.3	33
43	Chiral Recognition in Biomembrane Models: What is behind a â€˜Simple Modelâ€™. Synlett, 2009, 2009, 1023-1033.	1.0	3
44	Noble gasâ€“selenium molecular species: A theoretical investigation of FNgSeâ^' (Ng=Heâ€“Xe). Chemical Physics Letters, 2009, 470, 49-53.	1.2	18
45	Positive Ion Chemistry of SiH4/NF3 Gaseous Mixtures Studied by Ion Trap Mass Spectrometry. European Journal of Mass Spectrometry, 2009, 15, 209-220.	0.5	7
46	Cl-Initiated oxidation of N-ethyl-perfluoroalkanesulfonamides: A theoretical insight into the experimentally observed products. Computational and Theoretical Chemistry, 2008, 857, 57-65.	1.5	1
47	Ion chemistry in germane/fluorocompounds gaseous mixtures: a mass spectrometric and theoretical study. Journal of Mass Spectrometry, 2008, 43, 1320-1333.	0.7	11
48	Noble gasâ€“sulfur anions: A theoretical investigation of FNgSâ^' (Ng=He, Ar, Kr, Xe). Chemical Physics Letters, 2008, 458, 48-53.	1.2	29
49	Chiral recognition of dipeptides in bio-membrane models: the role of amphiphile hydrophobic chains. Tetrahedron: Asymmetry, 2008, 19, 124-130.	1.8	13
50	Noble Gas Anions:â€‰ A Theoretical Investigation of FNgBN⁻(Ng = Heâ^'Xe). Journal of Physical Chemistry A, 2007, 111, 10144-10151.	1.1	53
51	Nobleâ€Gas Complexes: Theoretical Investigation of Multicenter Polynuclear Species. Helvetica Chimica Acta, 2007, 90, 1335-1352.	1.0	4
52	Gas-phase ion chemistry of NF3/SO2 mixtures: A mass spectrometric and theoretical investigation. International Journal of Mass Spectrometry, 2007, 266, 86-91.	0.7	2
53	Role of the Spacer Stereochemistry on the Aggregation Properties of Cationic Gemini Surfactants. Langmuir, 2006, 22, 9333-9338.	1.6	36
54	Ge3Hn-Anions (n= 0â^'5) and Their Neutral Analogues:Â A Theoretical Investigation on the Structure, Stability, and Thermochemistry. Journal of Physical Chemistry A, 2006, 110, 9429-9437.	1.1	3

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55	Cationic Germanium Fluorides:Â A Theoretical Investigation on the Structure, Stability, and Thermochemistry of GeFn/GeFn+(n= 1â˜3). Journal of Physical Chemistry A, 2006, 110, 4900-4905.	1.1	15
56	Ligation of Be+ and Mg+ to NF3: Structure, stability, and thermochemistry of the Be+â€“(NF3) and Mg+â€“(NF3) complexes. International Journal of Mass Spectrometry, 2006, 255-256, 11-19.	0.7	4
57	Chiral recognition of dipeptides in phosphatidylcholine aggregates. Tetrahedron: Asymmetry, 2006, 17, 2731-2737.	1.8	14
58	Cationic germanium fluorides. International Journal of Mass Spectrometry, 2006, 257, 50-59.	0.7	8
59	Neutral Helium Compounds: Theoretical Evidence for a Large Class of Polynuclear Complexes. Chemistry - A European Journal, 2006, 12, 5033-5042.	1.7	36
60	Fluoromethyl Cations and Group XIV Congeners AHnF3 â€“n+ (A = Si, Ge, Sn, Pb;n = 0â€“2): From Covalent Structures to Ion-Molecule Complexes. European Journal of Inorganic Chemistry, 2006, 2006, 3010-3015.	1.0	5
61	From OBeHe to H3BOBeHe: Enhancing the stability of a neutral helium compound. Chemical Physics Letters, 2005, 406, 179-183.	1.2	43
62	Role of the Spacer of Cationic Gemini Amphiphiles in the Condensation of DNA. Langmuir, 2005, 21, 10271-10274.	1.6	62
63	Comment on â€œComputational Investigation of SO3â˜NH3-nXn(n= 0â˜3; X = F, Cl) Interactionsâ€• Journal of Physical Chemistry A, 2005, 109, 2410-2411.	1.1	1
64	New biphenylic derivatives: synthesis, characterisation and enantiodiscrimination in chiral aggregates. Tetrahedron: Asymmetry, 2004, 15, 987-994.	1.8	24
65	Nitrogen Trifluoride as a Bifunctional Lewis Base: Implications for the Adsorption of NF3 on Solid Surfaces. European Journal of Inorganic Chemistry, 2004, 2004, 1125-1130.	1.0	11
66	A Computational Investigation of HCN2+ Isomeric Structures: Implications for the Chemistry of Titan's Atmosphere. ChemPhysChem, 2004, 5, 1345-1351.	1.0	3
67	FN+Cl Ions from Ionized F2NCl: a Computational Investigation on the Structure and Reactivity toward H2O. Helvetica Chimica Acta, 2004, 87, 1467-1482.	1.0	3
68	Elucidation of the isomeric domains formed by sodium N-dodecanoyl-l-prolinate. Journal of Colloid and Interface Science, 2004, 280, 212-218.	5.0	2
69	SBeNg, SBNg+, and SCNg2+ complexes (Ng=He, Ne, Ar): a computational investigation on the structure and stability. Chemical Physics Letters, 2004, 384, 25-29.	1.2	38
70	OBHe+: a remarkably stable singly charged cation containing helium. Chemical Physics Letters, 2004, 398, 357-360.	1.2	6
71	Chiral Recognition of Dipeptides in a Biomembrane Model. Journal of the American Chemical Society, 2004, 126, 13354-13362.	6.6	50
72	Deracemization of an axially chiral biphenylic derivative as a tool for investigating chiral recognition in self-assemblies. Chirality, 2003, 15, 441-447.	1.3	29

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73	Surface Charge Density Determines the Efficiency of Cationic Gemini Surfactant Based Lipofection. Biophysical Journal, 2003, 84, 578-587.	0.2	55
74	Spectroscopic studies on the selective inclusion of amphiphilised porphyrin derivatives in micellar phases. Journal of Porphyrins and Phthalocyanines, 2003, 07, 181-190.	0.4	7
75	Effect of surfactant phase transition on the inclusion behaviour of an amphiphilised porphyrin derivativeElectronic supplementary information (ESI) available: experimental details of spectroscopic studies. See http://www.rsc.org/suppdata/cc/b1/b111692d/The synthesis of porphyrin 1 is described in ref. 8. Brij 35 and CTAN stand for polyoxyethylene(23)lauryl ether, and cetyltrimethylammonium nitrate, respectively. Critical Micelle Concentration (cmc) of Brij 35 is 0.05 mM (see ref. 11); that of CTAN is 0.8 mM. Chemical Communications, 2002, , 774-775.	2.2	7
76	Title is missing!. Helvetica Chimica Acta, 2002, 85, 2817-2826.	1.0	6
77	Structural effects on the NaOCl epoxidation of styrene in micellar media catalysed by amphiphilised Mn(III)metalloporphyrins. Journal of Molecular Catalysis A, 2002, 179, 125-131.	4.8	19
78	Selectivity in the Oxidation of Limonene by Amphiphilized Metalloporphyrins in Micellar Media. Langmuir, 2001, 17, 7198-7203.	1.6	29
79	Characterization of Mixed Monolayers of Phosphatidylcholine and a Dicationic Gemini Surfactant SS-1 with a Langmuir Balance: Effects Of DNA. Biophysical Journal, 2001, 81, 2135-2143.	0.2	41
80	Conformational Behavior of Aqueous Micelles of Sodium N-Dodecanoyl-l-prolinate. Langmuir, 1999, 15, 2627-2630.	1.6	24
81	Recognition in Organized Aggregates Formed by a Chiral Amidic Surfactant. Langmuir, 1999, 15, 8025-8031.	1.6	31
82	Deracemization of an Axially Chiral Biphenylic Structure in Chiral Micellar Aggregates. Langmuir, 1998, 14, 1960-1962.	1.6	20