Otilia Mo Romero

List of Publications by Year
in descending order

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368 papers	9,510 citations	41258 49 h-index	79541 73 g-index
376 all docs	376 docs citations	376 times ranked	4327 citing authors

#	Article	IF	Citations
1	A Theoretical Survey of the UVâ€“Visible Spectra of Axially and Peripherally Substituted Boron Subphthalocyanines. Computation, 2022, 10, 14.	1.0	3
2	Malonaldehyde-like Systems: BeF2 Clustersâ€”A Subtle Balance between Hydrogen Bonds, Beryllium Bonds, and Resonance. Sci, 2022, 4, 7.	1.8	0
3	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	1.3	3
4	Perturbating Intramolecular Hydrogen Bonds through Substituent Effects or Non-Covalent Interactions. Molecules, 2021, 26, 3556.	1.7	6
5	Clustering of Electron Deficient Bâ€•and Beâ€Containing Analogues: In the Fight for Tetracoordination, Beryllium Takes the Lead. European Journal of Inorganic Chemistry, 2021, 2021, 4393-4401.	1.0	2
6	Significant bonding rearrangements triggered by Mg4 clusters. Journal of Chemical Physics, 2021, 154, 044302.	1.2	2
7	Enthalpies of Adduct Formation between Boron Trifluoride and Selected Organic Bases in Solution: Toward an Accurate Theoretical Entry to Lewis Basicity. Molecules, 2021, 26, 6659.	1.7	7
8	Some interesting features of the rich chemistry around electron-deficient systems. Pure and Applied Chemistry, 2020, 92, 773-787.	0.9	3
9	The Importance of Strain (Preorganization) in Beryllium Bonds. Molecules, 2020, 25, 5876.	1.7	2
10	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in Xâ€“Yâ€“X (X = B, Al;) Tj ETQq0 0 0 rgBT /Overlock	1.4	2
11	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. Journal of Physical Chemistry A, 2020, 124, 5871-5878.	1.1	13
12	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. Journal of Physical Chemistry A, 2020, 124, 1515-1521.	1.1	3
13	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. Journal of Physical Chemistry A, 2019, 123, 7124-7132.	1.1	24
14	Combined Experimental and Theoretical Survey of the Gas-Phase Reactions of Serineâ€“Ca²⁺ Adducts. Journal of Physical Chemistry A, 2019, 123, 6241-6250.	1.1	5
15	On the Lewis Basicity of Phosphoramides: A Critical Examination of Their Donor Number through Comparison of Enthalpies of Adduct Formation with SbCl 5 and BF 3. ChemPhysChem, 2019, 20, 2566-2576.	1.0	6
16	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	0.4	36
17	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	1.3	13
18	Ternary Complexes Stabilized by Chalcogen and Alkalineâ€Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions. Chemistry - A European Journal, 2019, 25, 11688-11695.	1.7	20

#	Article	IF	Citations
19	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	5
20	Alkylation of uracil and thymine in the gas phase through interaction with alkylmercury compounds. International Journal of Mass Spectrometry, 2019, 436, 153-165.	0.7	5
21	Complexes between H₂ and neutral oxyacid beryllium derivatives. The role of angular strain. Molecular Physics, 2019, 117, 1142-1150.	0.8	5
22	Beâ€•and Mgâ€Based Electron and Anion Sponges. ChemPhysChem, 2018, 19, 1701-1706.	1.0	8
23	Trapping One Electron between Three Beryllium Atoms: Very Strong Oneâ€Electron Threeâ€Center Bonds. ChemPhysChem, 2018, 19, 1068-1074.	1.0	6
24	Alkaline-earth (Be, Mg and Ca) bonds at the origin of huge acidity enhancements. Physical Chemistry Chemical Physics, 2018, 20, 2413-2420.	1.3	32
25	Are beryllium-containing biphenyl derivatives efficient anion sponges?. Journal of Molecular Modeling, 2018, 24, 16.	0.8	7
26	Large Protonâ€Affinity Enhancements Triggered by Noncovalent Interactions. Chemistry - A European Journal, 2018, 24, 1971-1977.	1.7	15
27	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. Dalton Transactions, 2018, 47, 12516-12520.	1.6	7
28	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	8
29	Publications of Manuel YÃ¡Ã±ez and Otilia MÃ³. Journal of Physical Chemistry A, 2018, 122, 5681-5697.	1.1	1
30	Complexes between cyclopentene and cyclopentyne derivatives with HCu and FCu: The importance of cyclization effects. International Journal of Quantum Chemistry, 2018, 118, e25489.	1.0	1
31	Characterizing magnesium bonds: main features of a non-covalent interaction. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	21
32	Oneâ€Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. Angewandte Chemie, 2017, 129, 6892-6896.	1.6	8
33	Oneâ€Electron Bonds in Frustrated Lewis Pair TPB Ligands: Boron Behaving as a Lewis Base. Angewandte Chemie - International Edition, 2017, 56, 6788-6792.	7.2	11
34	Formation of unexpected silicon- and disiloxane-bridged multiferrocenyl derivatives bearing Siâ€“Oâ€“CHî€CH₂ and Siâ€“(CH₂)₂C(CH₃)₃ substituents via cleavage of tetrahydrofuran and trapping of its ring fragments. Dalton Transactions, 2017, 46, 11584-11597.	1.6	5
35	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	1.3	10
36	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie - International Edition, 2016, 55, 8736-8739.	7.2	22

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37	On the existence of intramolecular one-electron Beâ€“Be bonds. Chemical Communications, 2016, 52, 9656-9659.	2.2	28
38	Gasâ€Phase Infrared Spectroscopy of Substituted Cyanobutadiynes: Roles of the Bromine Atom and Methyl Group as Substituents. ChemPhysChem, 2016, 17, 1018-1024.	1.0	8
39	Exergonic and Spontaneous Production of Radicals through Beryllium Bonds. Angewandte Chemie, 2016, 128, 8878-8881.	1.6	9
40	Multi-Ferrocene-Containing Silanols as Redox-Active Anion Receptors. Organometallics, 2016, 35, 3507-3519.	1.1	12
41	Boronâ€Boron Oneâ€Electron Sigma Bonds versus Bâ€Xâ€B Bridged Structures. Chemistry - A European Journal, 2016, 22, 13697-13704.	1.7	13
42	Beryllium subphthalocyanines self-assembling properties. Canadian Journal of Chemistry, 2016, 94, 1015-1021.	0.6	3
43	Berylliumâ€Based Anion Sponges: Close Relatives of Proton Sponges. Chemistry - A European Journal, 2016, 22, 18322-18325.	1.7	24
44	Effect of beryllium bonds on the ketoâ€“enol tautomerism of formamide derivatives: a subtle basicityâ€“acidity balance. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
45	Fullerene and corannulene derivatives acting as insulators of Cl^{â^’}and BeH₂. Physical Chemistry Chemical Physics, 2016, 18, 6059-6068.	1.3	5
46	Photochemical Behavior of Beryllium Complexes with Subporphyrazines and Subphthalocyanines. Journal of Physical Chemistry A, 2016, 120, 4845-4852.	1.1	12
47	Aluminum Monocation Basicity and Affinity Scales. European Journal of Mass Spectrometry, 2015, 21, 517-532.	0.5	8
48	Simultaneous Aromaticâ€“Beryllium Bonds and Aromaticâ€“Anion Interactions: Naphthalene and Pyrene as Models of Fullerenes, Carbon Singleâ€Walled Nanotubes, and Graphene. ChemPhysChem, 2015, 16, 2680-2686.	1.0	8
49	Ga⁺ Basicity and Affinity Scales Based on Highâ€Level Abâ€…Initio Calculations. ChemPhysChem, 2015, 16, 3206-3213.	1.0	0
50	Creating Ïƒâ€Holes through the Formation of Beryllium Bonds. Chemistry - A European Journal, 2015, 21, 12676-12682.	1.7	38
51	Why Is the Spontaneous Deprotonation of [Cu(uracil)₂]²⁺ Complexes Accompanied by Enolization of the System?. ChemPhysChem, 2015, 16, 2375-2382.	1.0	2
52	Effects of the ionization in the tautomerism of uracil: A reaction electronic flux perspective. Journal of Computational Chemistry, 2015, 36, 2135-2145.	1.5	6
53	Interplay between Beryllium Bonds and Anion-Ï€ Interactions in BeR2:C6X6:Yâ^’ Complexes (R = H, F and Cl,) Tj ETQq1 1 0.784314 rgBT	1.7	11
54	Ferrocene and Silicon-Containing Oxathiacrown Macrocycles and Linear Oligo-Oxathioethers Obtained via Thiolâ€“Ene Chemistry of a Redox-Active Bifunctional Vinyldisiloxane. Macromolecules, 2015, 48, 6955-6969.	2.2	14

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55	Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds. Physical Chemistry Chemical Physics, 2015, 17, 2259-2267.	1.3	49
56	Intervalence charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds. Computational and Theoretical Chemistry, 2015, 1053, 281-288.	1.1	5
57	Acidity enhancement of unsaturated bases of group 15 by association with borane and beryllium dihydride. Unexpected boron and beryllium BrÅ¸nsted acids. Dalton Transactions, 2015, 44, 1193-1202.	1.6	17
58	Can Transition Metals and Group II Mono- and Dications Discriminate between Homo- and Heterochiral XYYXâ€™ Dimers (X,Xâ€™=H,Me; Y=O,S,Se)?. Croatica Chemica Acta, 2014, 87, 481-493.	0.1	1
59	Some Interesting Features of Non-Covalent Interactions. Croatica Chemica Acta, 2014, 87, 291-306.	0.1	14
60	New insights into the gas-phase unimolecular fragmentations of [Cysteineâ€“Ca]2+ complexes. Computational and Theoretical Chemistry, 2014, 1047, 38-46.	1.1	2
61	On the Structures, Lifetimes, and Infrared Spectra of Alkylmercury Hydrides. ChemPhysChem, 2014, 15, 530-541.	1.0	3
62	Spontaneous H₂ Loss through the Interaction of Squaric Acid Derivatives and BeH₂. Chemistry - A European Journal, 2014, 20, 5309-5316.	1.7	19
63	Changing Weak Halogen Bonds into Strong Ones through Cooperativity with Beryllium Bonds. Journal of Physical Chemistry A, 2014, 118, 4205-4213.	1.1	54
64	Cooperativity in beryllium bonds. Physical Chemistry Chemical Physics, 2014, 16, 4305-4312.	1.3	37
65	Spontaneous proton transfers induced by beryllium bonds. Molecular Physics, 2014, 112, 592-600.	0.8	30
66	On the existence and characteristics of Ï€-beryllium bonds. Physical Chemistry Chemical Physics, 2014, 16, 17531-17536.	1.3	34
67	Behavior of Carboxylic Acids upon Complexation with Beryllium Compounds. Journal of Physical Chemistry A, 2014, 118, 5720-5726.	1.1	9
68	Are Boryl Radicals from Amineâ€“Boranes and Phosphineâ€“Boranes the Most Stable Radicals?. ChemPhysChem, 2014, 15, 2288-2294.	1.0	4
69	On the stability of [Pb(Proline)]2+ complexes. Reconciling theory with experiment. Chemical Physics Letters, 2014, 598, 91-95.	1.2	6
70	Complexation of Ca2+ with selenocysteine and effects on its intrinsic acidity. Arkivoc, 2014, 2014, 207-223.	0.3	0
71	MS-CASPT2 study of the low-lying electronic excited states of di-thiosubstituted formic acid dimers. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	1
72	Alkyl mercury compounds: an assessment of DFT methods. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	19

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73	Can Conventional Bases and Unsaturated Hydrocarbons Be Converted into Gasâ€Phase Superacids That Are Stronger than Most of the Known Oxyacids? The Role of Beryllium Bonds. Chemistry - A European Journal, 2013, 19, 11637-11643.	1.7	55
74	Mechanochemical and silica gel-mediated formation of highly electron-poor 1-cyanocarbonylferrocene. Chemical Communications, 2013, 49, 9785.	2.2	15
75	Enhancing and modulating the intrinsic acidity of imidazole and pyrazole through beryllium bonds. Journal of Molecular Modeling, 2013, 19, 4139-4145.	0.8	34
76	Modulating weak intramolecular interactions through the formation of beryllium bonds: complexes between squaric acid and BeH2. Journal of Molecular Modeling, 2013, 19, 2759-2766.	0.8	24
77	Unimolecular Reactivity of the [Urea-Sr]2+ Complex, a Metastable Dication in the Gas Phase: An Experimental and Theoretical Perspective. Journal of Physical Chemistry B, 2013, 117, 2088-2095.	1.2	6
78	Spontaneous ion-pair formation in the gas phase induced by Beryllium bonds. Chemical Physics Letters, 2013, 590, 22-26.	1.2	30
79	Revealing Unexpected Mechanisms for Nucleophilic Attack on Sï£¿S and Seï£¿Se Bridges. Chemistry - A European Journal, 2013, 19, 3629-3638.	1.7	14
80	On the stability of [(uracil)2-Cu]2+ complexes in the gas phase. Different pathways for the formation of [(uracil-H)(uracil)-Cu]+ monocations. Organic and Biomolecular Chemistry, 2013, 11, 3862.	1.5	14
81	Resonance assisted hydrogen bonds in open-chain and cyclic structures of malonaldehyde enol: A theoretical study. Journal of Molecular Structure, 2013, 1048, 138-151.	1.8	28
82	Conformational preferences of RCH2CH2CN (RÂ=ÂCH3, F, Cl) cyanides and their corresponding isocyanides. Structural Chemistry, 2013, 24, 1789-1798.	1.0	3
83	Dramatic substituent effects on the mechanisms of nucleophilic attack on Se-S bridges. Journal of Computational Chemistry, 2013, 34, 2537-2547.	1.5	6
84	Modeling Interactions between an Amino Acid and a Metal Dication: Cysteineâ€“Calcium(II) Reactions in the Gas Phase. ChemPlusChem, 2013, 78, 1124-1133.	1.3	13
85	UV/Vis Spectra of Subporphyrazines and Subphthalocyanines with Aluminum and Gallium: A Timeâ€Dependent DFT Study. ChemPhysChem, 2013, 14, 915-922.	1.0	10
86	Infrared Spectra of Cyanoacetaldehyde (NCCH 2 CHO): A Potential Prebiotic Compound of Astrochemical Interest. ChemPhysChem, 2013, 14, 2764-2771.	1.0	7
87	Modelling peptideâ€“metal dication interactions: formamideâ€“Ca2+ reactions in the gas phase. Organic and Biomolecular Chemistry, 2012, 10, 7552.	1.5	16
88	Strong interactions between copper halides and unsaturated systems: new metallocycles? Or the importance of deformation. Physical Chemistry Chemical Physics, 2012, 14, 11468.	1.3	22
89	Cooperativity between hydrogen bonds and beryllium bonds in (H2O)nBeX2 (n = 1â€“3, X = H, F) complexes. A new perspective. Physical Chemistry Chemical Physics, 2012, 14, 14540.	1.3	67
90	Unexpected Acidity Enhancement Triggered by AlH₃ Association to Phosphines. Journal of Physical Chemistry A, 2012, 116, 6950-6954.	1.1	12

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91	Microsolvation of morpholine, a bidentate base â€“ the importance of cooperativity. Journal of Physical Organic Chemistry, 2012, 25, 1380-1390.	0.9	5
92	The importance of deformation on the strength of beryllium bonds. Computational and Theoretical Chemistry, 2012, 998, 74-79.	1.1	33
93	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. Journal of Chemical Theory and Computation, 2012, 8, 2293-2300.	2.3	81
94	Infrared spectra of chargeâ€solvated versus saltâ€bridge conformations of glycineâ€, serineâ€, and cysteineâ€Ca²⁺ complexes. International Journal of Quantum Chemistry, 2012, 112, 2126-2134.	1.0	9
95	On the Origin of the Enhanced Acidity of Chalcocyclopentadienes (Cyclopentadiene Chalcogenols) in the Gas Phase. ChemPhysChem, 2012, 13, 1167-1172.	1.0	3
96	Stability trends and tautomerization of chalcocyclopentadienes. The role of aromaticity. New Journal of Chemistry, 2011, 35, 2713.	1.4	4
97	TDDFT study of the UV-vis spectra of subporphyrazines and subphthalocyanines. Journal of Porphyrins and Phthalocyanines, 2011, 15, 1220-1230.	0.4	24
98	Modeling the interactions between peptide functions and Sr2+: formamideâ€“Sr2+ reactions in the gas phase. Physical Chemistry Chemical Physics, 2011, 13, 18409.	1.3	21
99	Effect of Sr²⁺association on the tautomerization processes of uracil and its dithio- and diseleno-derivatives. Organic and Biomolecular Chemistry, 2011, 9, 423-431.	1.5	9
100	La quÃmica computacional en la nueva frontera. Arbor, 2011, 187, 143-155.	0.1	0
101	Unimolecular reactivity upon collision of uracilâ€“Ca2+ complexes in the gas phase: Comparison with uracilâ€“M+ (M=H, alkali metals) and uracilâ€“M2+ (M=Cu, Pb) systems. International Journal of Mass Spectrometry, 2011, 306, 27-36.	0.7	37
102	Assisted intramolecular proton transfer in (uracil)2Ca2+ complexes. Theoretical Chemistry Accounts, 2011, 128, 457-464.	0.5	15
103	Unexpected Gas-Phase Ion Chemistry Results Unraveled by Computational Chemistry. Current Organic Chemistry, 2010, 14, 1600-1611.	0.9	6
104	New Insights into Factors Influencing Bï£¿N Bonding in X:BH_{3â^'n}F_nand X:BH_{3â^'n}Cl_nfor X=N₂, HCN, LiCN, H₂CNH, NF₃, NH₃andn=0â€“3: The Importance of Deformation. Chemistry - A European Journal, 2010, 16, 11897-11905.	1.7	39
105	Homoselenocysteine â€” An oxygen or selenium acid in the gas phase?. Canadian Journal of Chemistry, 2010, 88, 744-753.	0.6	2
106	The role of hyperconjugative ï€-aromaticity in the enhanced acidity of methyl-, silyl and germylcyclopentadienes. Molecular Physics, 2010, 108, 2467-2476.	0.8	7
107	Serineâ€“Ca²⁺versus serineâ€“Cu²⁺complexes â€” AÂtheoretical perspective. Canadian Journal of Chemistry, 2010, 88, 759-768.	0.6	11
108	Structural and Electronic Effects on One-Bond Spinâ^'Spin Coupling Constants1J(Bâ^'N),1J(Bâ^'H), and1J(Bâ^'F) for Complexes of Nitrogen Bases with BH3and Its Fluoro-Substituted Derivatives. Journal of Physical Chemistry A, 2010, 114, 12775-12779.	1.1	8

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109	Hydrogen bonding in electronically excited states: a comparison between formic acid dimer and its mono-substituted thioderivatives. Physical Chemistry Chemical Physics, 2010, 12, 13037.	1.3	8
110	Are cyclopentadienylberyllium, magnesium and calcium hydrides carbon or metal acids in the gas phase?. Dalton Transactions, 2010, 39, 4593.	1.6	11
111	Infrared Spectra of a Species of Potential Prebiotic and Astrochemical Interest: Cyanoethenethiol (NCâˆ’CHâ•CHâˆ’SH). Journal of Physical Chemistry A, 2010, 114, 9583-9588.	1.1	8
112	The mechanism of double proton transfer in dimers of uracil and 2â€thiouracilâ€”The reaction force perspective. Journal of Computational Chemistry, 2009, 30, 389-398.	1.5	26
113	A theoretical study of diborenes HLB=BLH for L=CO, NH3, OH2, PH3, SH2, ClH: structures, energies, and spinâ€“spin coupling constants. Theoretical Chemistry Accounts, 2009, 124, 187-195.	0.5	10
114	Beryllium Bonds, Do They Exist?. Journal of Chemical Theory and Computation, 2009, 5, 2763-2771.	2.3	158
115	The effects of C by N replacement on the hydrogen bonding of malonaldehyde: N-formylformimidic acid, N-(hydroxymethyl)formamide and related compounds. Physical Chemistry Chemical Physics, 2009, 11, 762-769.	1.3	15
116	Combined Experimental and Theoretical Study on Hydrogen-Bonded Complexes between Cyclic Ketones, Lactones, and Lactams with 3,4-Dinitrophenol. Journal of Physical Chemistry A, 2009, 113, 14711-14717.	1.1	10
117	Ni⁺ reactions with aminoacetonitrile, a potential prebiological precursor of glycine. Journal of Mass Spectrometry, 2008, 43, 317-326.	0.7	9
118	Strong Dissimilarities Between the Gasâ€Phase Acidities of Saturated and Î±,Î²â€Unsaturated Boranes and the Corresponding Alanes and Gallanes. Chemistry - A European Journal, 2008, 14, 2201-2208.	1.7	12
119	Bonding in Tropolone, 2â€Aminotropone, and Aminotroponimine: No Evidence of Resonanceâ€Assisted Hydrogenâ€Bond Effects. Chemistry - A European Journal, 2008, 14, 4225-4232.	1.7	80
120	Î±,Î²â€Unsaturated and Saturated Derivatives of Be, Mg, and Ca: Are They Carbon or Metal Acids in the Gas Phase?. Chemistry - A European Journal, 2008, 14, 10423-10429.	1.7	8
121	Why Are Selenouracils as Basic as but Stronger Acids than Uracil in the Gas Phase?. ChemPhysChem, 2008, 9, 1715-1720.	1.0	5
122	Computational study on the kinetics of the reaction between Ca2+ and urea. Chemical Physics Letters, 2008, 456, 156-161.	1.2	14
123	Conformational analysis, NMR properties and nitrogen inversion of N-substituted 1,3-oxazines. New Journal of Chemistry, 2008, 32, 2209.	1.4	6
124	The importance of the oxidative character of doubly charged metal cations in binding neutral bases. [Urea-M]2+ and [thiourea-M]2+ (M = Mg, Ca, Cu) complexes. Physical Chemistry Chemical Physics, 2008, 10, 3229.	1.3	39
125	Structures, Bonding, and One-Bond Bâˆ’N and Bâˆ’H Spinâˆ’Spin Coupling Constants for a Series of Neutral and Anionic Five-Membered Rings Containing BN Bonds. Journal of Chemical Theory and Computation, 2008, 4, 1869-1876.	2.3	5
126	Selenoureaâˆ’Ca²⁺Reactions in Gas Phase. Similarities and Dissimilarities with Urea and Thiourea. Journal of Physical Chemistry B, 2008, 112, 5479-5486.	1.2	26

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127	On the Bonding of Selenocyanates and Isoselenocyanates and Their Protonated Derivatives. Journal of Chemical Theory and Computation, 2008, 4, 1593-1599.	2.3	8
128	Gas-Phase Interaction of Calcium (Ca²⁺) with Seleno Derivatives of Uracil. Journal of Chemical Theory and Computation, 2008, 4, 1002-1011.	2.3	14
129	Interaction of Ca2+ with uracil and its thio derivatives in the gas phase. Organic and Biomolecular Chemistry, 2008, 6, 3695.	1.5	40
130	Accelerating charge transfer in a triphenylamineâ€“subphthalocyanine donorâ€“acceptor system. Chemical Communications, 2008, , 1759.	2.2	68
131	Ni⁺Reactions with Aminoacrylonitrile, A Species of Potential Astrochemical Relevance. Journal of Physical Chemistry A, 2008, 112, 10509-10515.	1.1	6
132	Resonance-Assisted Hydrogen Bonds:Â A Critical Examination. Structure and Stability of the Enols of Î²-Diketones and Î²-Enaminones. Journal of Physical Chemistry A, 2007, 111, 3585-3591.	1.1	142
133	A theoretical study of hydration effects on the prototropic tautomerism of selenouracils. Organic and Biomolecular Chemistry, 2007, 5, 3092.	1.5	22
134	Effect of Ni(ii), Cu(ii) and Zn(ii) association on the keto-enol tautomerism of thymine in the gas phase. Physical Chemistry Chemical Physics, 2007, 9, 2531-2537.	1.3	30
135	Spinâ^'Spin Coupling Constants for Iminoboranes RBNH, HBNR, and RBNR and Comparisons with Corresponding Isoelectronic Acetylenes RCCH and RCCR, for R = H, CH3, NH2, OH, and F. Journal of Chemical Theory and Computation, 2007, 3, 549-556.	2.3	8
136	Attacking Boron Nucleophiles:â€‰ NMR Properties of Five-Membered Diazaborole Rings. Journal of Physical Chemistry A, 2007, 111, 419-421.	1.1	14
137	Unusual substituent effects on the bonding of iminoboranes. Physical Chemistry Chemical Physics, 2007, 9, 3970-3977.	1.3	31
138	Activation of the Disulfide Bond and Chalcogenâ€“Chalcogen Interactions: An Experimental (FTICR) and Computational Study. Chemistry - A European Journal, 2007, 13, 1796-1803.	1.7	25
139	How Can a Carbon Atom Be Covalently Bound to Five Ligands? The Case of Si2(CH3)7+. Angewandte Chemie - International Edition, 2007, 46, 381-385.	7.2	24
140	Unimolecular Reactivity of Uracilâ€“Cu2+ Complexes in the Gas Phase. ChemPhysChem, 2007, 8, 181-187.	1.0	64
141	Gas-Phase Reactions Between Thiourea and Ca2+: New Evidence for the Formation of [Ca(NH3)]2+ and Other Doubly Charged Species. ChemPhysChem, 2007, 8, 1330-1337.	1.0	25
142	Nonâ€Resonanceâ€Assisted Hydrogen Bonding in Hydroxymethylene and Aminomethylene Cyclobutanones and Cyclobutenones and Their Nitrogen Counterparts.. ChemPhysChem, 2007, 8, 1950-1958.	1.0	82
143	Thermochemistry, bonding, and reactivity of Ni + and Ni 2+ in the gas phase. Mass Spectrometry Reviews, 2007, 26, 474-516.	2.8	36
144	Cyano substituent effects on enol and enethiol acidity and basicity: The protonation and deprotonation of 3-hydroxy-2-propenenitrile and its thio analogue. International Journal of Mass Spectrometry, 2007, 267, 125-133.	0.7	18

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145	Substituent Effects on Enthalpies of Formation of Nitrogen Heterocycles:â€‰ 2-Substituted Benzimidazoles and Related Compounds. Journal of Physical Chemistry A, 2006, 110, 2535-2544.	1.1	17
146	Gas-Phase Deprotonation of Uracilâ^'Cu2+ and Thiouracilâ^'Cu2+ Complexes. Journal of Physical Chemistry A, 2006, 110, 1943-1950.	1.1	69
147	An ab Initio Study of15Nâ^'11B Spinâ^'Spin Coupling Constants for Borazine and Selected Derivatives. Journal of Physical Chemistry A, 2006, 110, 9959-9966.	1.1	49
148	Reactions of F+(3P) and F+(1D) with Silicon Oxide. Possibility of Spin-Forbidden Processes. Journal of Physical Chemistry A, 2006, 110, 7130-7137.	1.1	0
149	Analysis of the bonding in XH3ï£¿Cu+ (Xï£¾B, Al, Ga) complexes. International Journal of Quantum Chemistry, 2006, 106, 659-663.	1.0	4
150	On the stability of non-conventional Ï€-complexes between Ni+ and toluene, phenyl-silane and phenyl-germane. Journal of Physical Organic Chemistry, 2006, 19, 495-502.	0.9	3
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