Cristina Trujillo

List of Publications by Year
in descending order

82 papers	1,531 citations	279798 23 h-index	361022 35 g-index
89 all docs	89 docs citations	89 times ranked	1265 citing authors

#	Article	IF	Citations
1	Intermolecular Weak Interactions in HTeXH Dimers (X=O, S, Se, Te): Hydrogen Bonds, Chalcogenâ€“Chalcogen Contacts and Chiral Discrimination. ChemPhysChem, 2012, 13, 496-503.	2.1	101
2	Competition and Interplay between Ïƒ-Hole and Ï€-Hole Interactions: A Computational Study of 1:1 and 1:2 Complexes of Nitryl Halides (O₂NX) with Ammonia. Journal of Physical Chemistry A, 2012, 116, 5199-5206.	2.5	86
3	Orthogonal interactions between nitryl derivatives and electron donors: pnictogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 14310.	2.8	75
4	Intramolecular pnicogen interactions in phosphorus and arsenic analogues of proton sponges. Physical Chemistry Chemical Physics, 2014, 16, 15900-15909.	2.8	60
5	Intramolecular Pnicogen Interactions in PHFï£¿(CH₂)_nï£¿PHF (n=2â€“6) Systems. ChemPhysChem, 2013, 14, 1656-1665.	2.1	50
6	Halogen, chalcogen and pnictogen interactions in (XNO₂)₂homodimers (X = F,) Tj ETQq0 0 0 rgBT /Overlock	2.8	47
7	Electron density shift description of non-bonding intramolecular interactions. Computational and Theoretical Chemistry, 2012, 991, 124-133.	2.5	43
8	Interaction of Ca2+ with uracil and its thio derivatives in the gas phase. Organic and Biomolecular Chemistry, 2008, 6, 3695.	2.8	40
9	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.	2.8	39
10	A theoretical study of the hydrogen bonding properties of H2BNH2: Some considerations on the basis set superposition error issue. Computational and Theoretical Chemistry, 2011, 967, 147-151.	2.5	38
11	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au₂:HX Complexes. ChemPhysChem, 2019, 20, 1572-1580.	2.1	38
12	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.	1.5	37
13	Weak interactions between hypohalous acids and dimethylchalcogens. Physical Chemistry Chemical Physics, 2012, 14, 9880.	2.8	36
14	Improvement of Anion Transport Systems by Modulation of Chalcogen Interactions: The influence of solvent. Journal of Physical Chemistry A, 2018, 122, 1369-1377.	2.5	35
15	Non-Covalent Interactions: Complexes of Guanidinium with DNA and RNA Nucleobases. Journal of Physical Chemistry B, 2013, 117, 11608-11616.	2.6	32
16	A Study of Ï€â€“Ï€ Stacking Interactions and Aromaticity in Polycyclic Aromatic Hydrocarbon/Nucleobase Complexes. ChemPhysChem, 2016, 17, 395-405.	2.1	31
17	Modulating intramolecular Pâ‹¯N pnictogen interactions. Physical Chemistry Chemical Physics, 2016, 18, 9148-9160.	2.8	29
18	A theoretical NMR study of the structure of benzynes and some of their carbocyclic and heterocyclic analogs. Tetrahedron, 2012, 68, 6548-6556.	1.9	28

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19	Resonance assisted hydrogen bonds in open-chain and cyclic structures of malonaldehyde enol: A theoretical study. Journal of Molecular Structure, 2013, 1048, 138-151.	3.6	28
20	A DFT mechanistic study of the organocatalytic asymmetric reaction of aldehydes and homophthalic anhydride. Chemical Communications, 2017, 53, 8874-8877.	4.1	27
21	Selenoureaâ^'Ca²⁺Reactions in Gas Phase. Similarities and Dissimilarities with Urea and Thiourea. Journal of Physical Chemistry B, 2008, 112, 5479-5486.	2.6	26
22	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.	2.1	25
23	Catalytic asymmetric Tamura cycloadditions involving nitroalkenes. Organic and Biomolecular Chemistry, 2017, 15, 1463-1474.	2.8	25
24	TDDFT study of the UV-vis spectra of subporphyrazines and subphthalocyanines. Journal of Porphyrins and Phthalocyanines, 2011, 15, 1220-1230.	0.8	24
25	A theoretical study of hydration effects on the prototropic tautomerism of selenouracils. Organic and Biomolecular Chemistry, 2007, 5, 3092.	2.8	22
26	Simultaneous Interactions of Anions and Cations with Cyclohexane and Adamantane: Aliphatic Cyclic Hydrocarbons as Charge Insulators. Journal of Physical Chemistry A, 2011, 115, 13124-13132.	2.5	20
27	Cooperative Effects in Weak Interactions: Enhancement of Tetrel Bonds by Intramolecular Hydrogen Bonds. Molecules, 2019, 24, 308.	3.8	20
28	Modulating intramolecular chalcogen bonds in aromatic (thio)(seleno)phene-based derivatives. Physical Chemistry Chemical Physics, 2019, 21, 23645-23650.	2.8	20
29	Theoretical study of cyanophosphines: Pnicogen vs. dipoleâ€“dipole interactions. Computational and Theoretical Chemistry, 2015, 1053, 305-314.	2.5	19
30	Thiophene/thiazole-benzene replacement on guanidine derivatives targeting Î± 2 -Adrenoceptors. European Journal of Medicinal Chemistry, 2017, 138, 38-50.	5.5	19
31	A theoretical study of the parent NH-benzazoles (benzimidazoles, indazoles and benzotriazoles): geometries, energies, acidity and basicity, NMR properties and molecular electrostatic potentials. Arkivoc, 2012, 2012, 85-107.	0.5	18
32	Computational Study of Proton Transfer in Tautomers of 3â€•and 5â€Hydroxypyrazole Assisted by Water. ChemPhysChem, 2015, 16, 2140-2150.	2.1	17
33	Solvent and Substituent Effects on the Phosphine + CO2 Reaction. Inorganics, 2018, 6, 110.	2.7	17
34	Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N2, OH2, NCH, SH2,) Tj ETQq0 0 0 rgBT /Overlock 1	2.2	17
35	Catalytic Asymmetric Î³â€Lactam Synthesis from Enolisable Anhydrides and Imines. Chemistry - A European Journal, 2019, 25, 7275-7279.	3.3	15
36	Evaluation of Electron Density Shifts in Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4741-4749.	2.5	15

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37	Divergent Pathways and Competitive Mechanisms of Metathesis Reactions between 3â€Arylpropâ€2â€ynyl Esters and Aldehydes: An Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 10360-10370.	3.3	14
38	Bisimidazoline arylamides binding to the DNA minor groove: N1-hydroxylation enhances binding affinity and selectivity to AATT sites. MedChemComm, 2015, 6, 2036-2042.	3.4	14
39	Catalytic Asymmetric Cycloadditions between Aldehydes and Enolizable Anhydrides: cis-Selective Dihydroisocoumarin Formation. Journal of Organic Chemistry, 2018, 83, 15499-15511.	3.2	13
40	Highly Enantioâ€•and Diastereoselective Catalytic Asymmetric Tamura Cycloaddition Reactions. Chemistry - A European Journal, 2019, 25, 7270-7274.	3.3	12
41	Discovery of a photochemical cascade process by flow-based interception of isomerising alkenes. Chemical Science, 2021, 12, 9895-9901.	7.4	12
42	A theoretical study on the aromaticity of benzene and related derivatives incorporating a Câ€“C Câ€“C fragment. Tetrahedron, 2013, 69, 7333-7344.	1.9	11
43	Aromatic Amino Acids-Guanidinium Complexes through Cation-Ï€ Interactions. Molecules, 2015, 20, 9214-9228.	3.8	11
44	A theoretical model of the interaction between phosphates in the ATP molecule and guanidinium systems. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	11
45	Enhancing Intramolecular Chalcogen Interactions in 1-Hydroxy-8-YH-naphthalene Derivatives. Journal of Physical Chemistry A, 2017, 121, 8995-9003.	2.5	11
46	Theoretical Investigation of Cyanoâ€Chalcogen Dimers and Their Importance in Molecular Recognition. ChemPhysChem, 2019, 20, 3186-3194.	2.1	11
47	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. ChemPhysChem, 2020, 21, 2557-2563.	2.1	11
48	The Lewis acidities of gold(I) and gold(III) derivatives: a theoretical study of complexes of AuCl and AuCl3. Structural Chemistry, 2020, 31, 1909-1918.	2.0	11
49	Influence of fluoro and cyano substituents in the aromatic and antiaromatic characteristics of cyclooctatetraene. Physical Chemistry Chemical Physics, 2015, 17, 14961-14971.	2.8	10
50	Improving phase-transfer catalysis by enhancing non-covalent interactions. Physical Chemistry Chemical Physics, 2020, 22, 21015-21021.	2.8	10
51	An insight on the aromatic changes in closed shell icosagen, tetrel, and pnictogen phenalenyl derivatives. Structural Chemistry, 2017, 28, 345-355.	2.0	9
52	Sequestration of CO₂ by Phosphatrane Molecules. ChemPhysChem, 2019, 20, 3195-3200.	2.1	9
53	The base-catalysed Tamura cycloaddition reaction: calculation, mechanism, isolation of intermediates and asymmetric catalysis. Chemical Communications, 2019, 55, 11283-11286.	4.1	9
54	On the Bonding of Selenocyanates and Isoselenocyanates and Their Protonated Derivatives. Journal of Chemical Theory and Computation, 2008, 4, 1593-1599.	5.3	8

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55	Competition between intramolecular hydrogen and pnictogen bonds in protonated systems. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	8
56	Weak interactions within nitryl halide heterodimers. New Journal of Chemistry, 2016, 40, 9060-9072.	2.8	8
57	Aromatic changes in isoelectronic derivatives of phenalenyl radicals by central carbon replacement. Tetrahedron, 2016, 72, 4690-4699.	1.9	8
58	An Insight into Nonâ€Covalent Interactions on the Bicyclo[1.1.1]pentane Scaffold. European Journal of Organic Chemistry, 2021, 2021, 1113-1122.	2.4	8
59	Thermodynamic and hydrogen-bond basicity of phosphine oxides: Effect of the ring strain. Computational and Theoretical Chemistry, 2012, 994, 81-90.	2.5	7
60	Structure, binding energy and chiral discrimination in oxathiirane homodimers. Computational and Theoretical Chemistry, 2016, 1090, 171-179.	2.5	7
61	Interaction between Trinuclear Regium Complexes of Pyrazolate and Anions, a Computational Study. International Journal of Molecular Sciences, 2020, 21, 8036.	4.1	7
62	A theoretical reappraisal of the cyclol hypothesis. Structural Chemistry, 2012, 23, 873-877.	2.0	6
63	Effect of isouronium/guanidinium substitution on the efficacy of a series of novel anti-cancer agents. MedChemComm, 2018, 9, 735-743.	3.4	6
64	Why Are Selenouracils as Basic as but Stronger Acids than Uracil in the Gas Phase?. ChemPhysChem, 2008, 9, 1715-1720.	2.1	5
65	A theoretical investigation of the mechanism of formation of a simplified analog of the green fluorescent protein (GFP) from a peptide model. Structural Chemistry, 2013, 24, 1145-1151.	2.0	5
66	The Steglich Rearrangement of 2â€Oxindole Derivatives Promoted by Anionâ€based Nucleophilic Catalysis. ChemCatChem, 2019, 11, 3776-3780.	3.7	5
67	Catalyst design within asymmetric organocatalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	5
68	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au 2 :HX Complexes. ChemPhysChem, 2019, 20, 1552-1552.	2.1	4
69	Planarity or Nonplanarity: Modulating Guanidine Derivatives as Î±2-Adrenoceptors Ligands. Journal of Chemical Information and Modeling, 2019, 59, 2479-2486.	5.4	4
70	Cyclohexane-Based Scaffold Molecules Acting as Anion Transport, Anionophores, via Noncovalent Interactions. Journal of Chemical Information and Modeling, 2019, 59, 2212-2217.	5.4	4
71	Modulation of in:out and out:out conformations in [X.Xâ€².Xâ€²â€²] phosphatranes by Lewis acids. Physical Chemistry Chemical Physics, 2017, 19, 20647-20656.	2.8	3
72	Anion Recognition by Neutral and Cationic Iodotriazole Halogen Bonding Scaffolds. Molecules, 2020, 25, 798.	3.8	3

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73	A Computational Study on 3â€Azoniaâ€ 3â€Phosphoniaâ€ and 3â€Arsoniaspiro[2.2]pentanes and Related Threeâ€Membered Heterocycles. ChemPhysChem, 2014, 15, 3493-3501.	2.1	2
74	Development of the first model of a phosphorylated, ATP/Mg²⁺-containing B-Raf monomer by molecular dynamics simulations: a tool for structure-based design. Physical Chemistry Chemical Physics, 2017, 19, 31177-31185.	2.8	2
75	Study of Meldrumâ€™s Acid Cyclization Reactions. Journal of Physical Chemistry A, 2018, 122, 2535-2541.	2.5	2
76	Dual-binding conjugates of diaromatic guanidines and porphyrins for recognition of G-quadruplexes. Organic and Biomolecular Chemistry, 2020, 18, 5617-5624.	2.8	2
77	Ca2+ Reactivity in the Gas Phase. Bonding, Catalytic Effects and Coulomb Explosions. Challenges and Advances in Computational Chemistry and Physics, 2010, , 1-33.	0.6	2
78	Kinetical and thermodynamical analysis of the reactivity of thiourea by association to Ca2+. Computational and Theoretical Chemistry, 2015, 1052, 68-72.	2.5	1
79	Reactivity of Coinage Metal Hydrides for the Production of H 2 Molecules. ChemistryOpen, 2021, 10, 724-730.	1.9	1
80	Reactions of F+(3P) and F+(1D) with Silicon Oxide. Possibility of Spin-Forbidden Processes. Journal of Physical Chemistry A, 2006, 110, 7130-7137.	2.5	0
81	Reactivity of Coinage Metal Hydrides for the Production of H 2 Molecules. ChemistryOpen, 2021, 10, 722-723.	1.9	0
82	Mechanistic Insights into the Organocatalytic Kinetic Resolution of Oxazinones via Alcoholysis. European Journal of Organic Chemistry, 2022, 2022, e202100818.	2.4	0