Boaz Oliveira

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2377091/publications.pdf

Version: 2024-02-01

64	1,295	257450	377865
papers	citations	24 h-index	34 g-index

65	65	65	718
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The hydrogen bond strength: New proposals to evaluate the intermolecular interaction using DFT calculations and the AIM theory. Chemical Physics Letters, 2006, 427, 181-184.	2.6	99
2	Design, synthesis and cruzain docking of 3-(4-substituted-aryl)-1,2,4-oxadiazole-N-acylhydrazones as anti-Trypanosoma cruzi agents. Bioorganic and Medicinal Chemistry, 2009, 17, 6682-6691.	3.0	84
3	Structure, energy, vibrational spectrum, and Bader's analysis of Ï€â‹¯H hydrogen bonds and H^{â‹¯Î´}â‹¯H^{+Î´}dihydrogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 37-79.	2.8	63
4	Hydrogen bonds in alcohols:water complexes: A theoretical study about new intramolecular interactions via CHELPG and AIM calculations. Computational and Theoretical Chemistry, 2006, 774, 83-88.	1.5	57
5	The Use of Solid Dispersion Systems in Hydrophilic Carriers to Increase Benznidazole Solubility. Journal of Pharmaceutical Sciences, 2011, 100, 2443-2451.	3.3	53
6	A theoretical study of blue-shifting hydrogen bonds in Ï€ weakly bound complexes. Computational and Theoretical Chemistry, 2009, 908, 79-83.	1.5	38
7	A theoretical study of red-shifting and blue-shifting hydrogen bonds occurring between imidazolidine derivatives and PEG/PVP polymers. Journal of Molecular Modeling, 2010, 16, 119-127.	1.8	38
8	The molecular properties of heterocyclic and homocyclic hydrogen-bonded complexes evaluated by DFT calculations and AIM densities. Journal of Molecular Modeling, 2009, 15, 123-131.	1.8	37
9	The hydrogen bond in the acetylene-2(HF) complex: A theoretical study about intramolecular and unusual Ï€â‹¯H interactions using DFT and AIM calculations. Computational and Theoretical Chemistry, 2006, 775, 39-45.	1.5	35
10	Uncommon hydrogen bonds between a non-classical ethyl cation and Ï€ hydrocarbons: a preliminary study. Structural Chemistry, 2009, 20, 81-90.	2.0	34
11	Multiple proton donors on BeH2Â·Â·Â·2HCl trimolecular dihydrogen-bonded complex: some theoretical insights. Structural Chemistry, 2008, 19, 665-670.	2.0	33
12	Interplay between dihydrogen and alkaliâ€“halogen bonds: Is there some covalency upon complexation of ternary systems?. Computational and Theoretical Chemistry, 2012, 998, 173-182.	2.5	33
13	Synthesis and conformational study of a new class of highly bioactive compounds. Chemical Physics Letters, 2007, 449, 336-340.	2.6	31
14	Dihydrogen bonds and blueâ€shifting hydrogen bonds: A theoretical study of AHÂ·Â·Â·HCF₃and TH₂Â·Â·Â·HCF₃model systems with A = Li or Na and T = Be or Mg. International Journal of Quantum Chemistry, 2010, 110, 307-316.	2.0	30
15	Theoretical study of cooperative effects in the homo- and heteromeric hydrogen bond chains (HCN)nï£¿HF withn = 1, 2, and 3. International Journal of Quantum Chemistry, 2006, 106, 2714-2722.	2.0	29
16	RelaÃ§Ã£o entre transferÃªncia de carga e as interaÃ§Ãµes intermoleculares em complexos de hidrogÃªnio heterocÃ¢licos. Quimica Nova, 2007, 30, 791-796.	0.3	28
17	Small heterocyclics as hydrogen bond acceptors and donors: the case of the C2H3XSÂ·Â·Â·NH3 complexes (XÂ=ÂH, F and CH3). Structural Chemistry, 2009, 20, 663-670.	2.0	28
18	A topologia molecular QTAIM e a descriÃ§Ã£o mecÃ¢nico-quÃ¢ntica de ligaÃ§Ãµes de hidrogÃªnio e ligaÃ§Ãµes de di-hidrogÃªnio. Quimica Nova, 2010, 33, 1155-1162.	0.3	28

#	Article	IF	Citations
19	A theoretical study of the solvent effects in ethylene oxide: Hydrofluoric acid complex using continuum and new discrete models. Computational and Theoretical Chemistry, 2007, 802, 91-97.	1.5	27
20	The (H-Î´Â·Â·Â·H+Î´) charge transfer and the evaluation of the harmonic molecular properties of dihydrogen-bonded complexes formed by BeH2Â·Â·Â·HX with XÂ=ÂF, Cl, CN, and CCH. Structural Chemistry, 2008, 19, 185-189.	2.0	27
21	A B3LYP and QTAIM study of a new proton donor for dihydrogen bonds: the case of the C2H5 +Â·Â·Â·nBeH2 complexes (nÂ=Â1 or 2). Structural Chemistry, 2009, 20, 897-902.	2.0	27
22	A theoretical study of three and four proton donors on linear HXÂ·Â·Â·BeH2Â·Â·Â·HX and bifurcate BeH2Â·Â·Â·2HX trimolecular dihydrogen-bonded complexes with XÂ=ÂCN and NC. Structural Chemistry, 2010, 21, 221-228.	2.0	26
23	Um estudo teÃ³rico de propriedades moleculares em complexos de hidrogÃªnio trimoleculares C2H4Â·Â·Â·2HF, C2H2Â·Â·Â·2HF e C3h6Â·Â·Â·2HF. Quimica Nova, 2008, 31, 1673-1679.	0.3	24
24	A quantum chemical study of red-shift and blue-shift hydrogen bonds in bimolecular and trimolecular methylhydrazine-hydrate complexes. Computational and Theoretical Chemistry, 2009, 915, 38-42.	1.5	24
25	A chemometrical study of intermolecular properties of hydrogen-bonded complexes formed by C2H4Oâ‹…â‹…â‹…HX and C2H5Nâ‹…â‹…â‹…HX with X = F, CN, NC, and CCH. Journal of Molecular Modeling, 2009, 15, 421-432.	1.8	23
26	An energetic quantification of interâ€“intramolecular interactions in the C2H2â€“2HF and C2H4Oâ€“2HF trimolecular hydrogen bonded complexes: DFT calculations and AIM topological parameters. Chemical Physics Letters, 2007, 433, 390-394.	2.6	22
27	A theoretical analysis of topography and molecular parameters of the CFCl₃Â·Â·Â·O₃ complex: Linear and bifurcate halogenâ€¢oxygen bonding interactions. International Journal of Quantum Chemistry, 2011, 111, 111-116.	2.0	22
28	The ethyl cation as proton donor for dihydrogen bonds in the (m=1 or 2 and n=1 or 2) complex: A theoretical study. Inorganic Chemistry Communication, 2009, 12, 1142-1144.	3.9	21
29	Evidence for blue-shifting and red-shifting effects in the C2H4Â·Â·Â·HCF3, C2H3(CH3)Â·Â·Â·HCF3 and C2H2(CH3)2Â·Â·Â·HCF3 complexes: Ï€ and improper-Ï€ hydrogen bonds. Computational and Theoretical Chemistry, 2010, 944, 168-172.	1.5	21
30	Frequency shifts and interaction strength of model hydrogen-bonded systems: new NBO and QTAIM characteristics. Structural Chemistry, 2014, 25, 745-753.	2.0	20
31	Um estudo teÃ³rico relativo Ã nÃ£o-linearidade da ligaÃ§Ã£o de hidrogÃªnio em sistemas heterocÃclicos C2H4O-C2H2 e C2H4S-C2H2. Quimica Nova, 2007, 30, 1167-1170.	0.3	18
32	A theoretical study of dihydrogen bonds in small protonated rings: Aziridine and azetidine cations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 563-566.	3.9	17
33	Theoretical aspects of binary and ternary complexes of aziridineâ‹¯ammonia ruled by hydrogen bond strength. Journal of Molecular Modeling, 2012, 18, 2845-2854.	1.8	16
34	Hydrogen bonds determine the structures of the ternary heterocyclic complexes C2H4OÂ·Â·Â·2HF, C2H5NÂ·Â·Â·2HF and C2H4SÂ·Â·Â·2HF: density functional theory and topological calculations. Journal of Molecular Modeling, 2011, 17, 2847-2862.	1.8	15
35	Theoretical estimation of pnicogen bonds and hydrogen bonds in small heterocyclic complexes: Red-shifts and blue-shifts ruled by polarization effects. Chemical Physics, 2014, 443, 67-75.	1.9	15
36	Bonding topology, hydrogen bond strength, and vibrational chemical shifts on hetero-ring hydrogen-bonded complexesÂâ€" Theoretical insights revisited. Canadian Journal of Chemistry, 2012, 90, 368-375.	1.1	13

#	Article	IF	Citations
37	The topology of Ï€Â·Â·Â·H hydrogen bonds. Monatshefte FÃ¼r Chemie, 2011, 142, 861-873.	1.8	12
38	Synthesis, anti-proliferative activity, theoretical and 1H NMR experimental studies of Moritaâ€“Baylisâ€“Hillman adducts from isatin derivatives. Molecular Diversity, 2020, 24, 265-281.	3.9	12
39	A new theoretical analysis of the cooperative effect in T-shaped hydrogen complexes of CnHmâˆ™âˆ™âˆ™HCNâˆ™âˆ™âˆ™HW with nâ€‰=â€‰2, mâ€‰=â€‰2 or 4, and Wâ€‰=â€‰F or CN. Journal of Molecular Modeling, 2013, 19, 3551-3568.	1.8	10
40	New insights about the hydrogen bonds formed between acetylene and hydrogen fluoride: Ï€ â‹¯ H, C â‹¯ H and F â‹¯ H. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 160-169.	3.9	10
41	Quantum chemical studies of non-covalent interactions between the ethyl cation and rare gases. Comptes Rendus Chimie, 2014, 17, 1041-1049.	0.5	9
42	The electronic mechanism ruling the dihydrogen bonds and halogen bonds in weakly bound systems of H3SiHÂ·Â·Â·HOX and H3SiHÂ·Â·Â·XOH (X = F, Cl, and Br). Journal of Molecular Modeling, 2015, 21, 77.	1.8	8
43	The interaction strengths and spectroscopy parameters of the C2H2âˆ™âˆ™âˆ™HX and HCNâˆ™âˆ™âˆ™HX complexes (X = F,) Tj ETQq1 NBO calculations. Journal of Molecular Modeling, 2017, 23, 110.	1.8	8
44	The acidity of analogous ammonium cations: A description of the solvent effect through the attainment of hydration clusters using the AGOA methodology. Computational and Theoretical Chemistry, 2008, 860, 13-17.	1.5	7
45	SAPT: ligaÃ§Ã£o de hidrogÃªnio ou interaÃ§Ã£o de van der Waals?. Quimica Nova, 2012, 35, 2002-2012.	0.3	7
46	The structures of heterocyclic complexes ruled by hydrogen bonds and halogen interactions: Interaction strength and IR modes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 124, 208-215.	3.9	7
47	A computational study of hydrogen bonds in intermolecular systems of high complexity: arachno-pentaborane(11)Â·Â·Â·Y with Yâ€‰=â€‰O2 and N2. Journal of Molecular Modeling, 2014, 20, 2403.	1.8	7
48	A quantum chemical study of molecular properties and QSPR modeling of oximes, amidoximes and hydroxamic acids with nucleophilic activity against toxic organophosphorus agents. Journal of Molecular Structure, 2017, 1133, 338-347.	3.6	7
49	The interplay and strength of the Ï€â‹¯H F, Câ‹¯H F, Fâ‹¯H F and Fâ‹¯H C hydrogen bonds upon the formation of multimolecular complexes based on C2H2â‹¯HF and C2H4â‹¯HF small dimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 213, 438-455.	3.9	7
50	The formation of HÂ·Â·Â·X hydrogen bond, CÂ·Â·Â·X carbon-halide or SiÂ·Â·Â·X tetrel bonds on the silylene-halogen dimers (Xâ€‰=â€‰F or Cl): intermolecular strength, molecular orbital interactions and prediction of covalency. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
51	The electronic donation and frequency shifts on the YCCHâ‹¯BH 4 â‹¯ boron-bonded complexes (Y = H, CH 3) Tj ETQq1 1 0.784314 rgB 580-587.	3.9	5
52	A comparative interplay between small heterorings and hypofluorous acids. Journal of Molecular Modeling, 2015, 21, 286.	1.8	4
53	Comparisons between Crystallography Data and Theoretical Parameters and the Formation of Intramolecular Hydrogen Bonds: Benznidazole. Crystals, 2016, 6, 56.	2.2	4
54	The interaction strength of intermolecular systems formed by NaHâ‹¯2(HF) and NaHâ‹¯4(HF): Hydrogen bonds, dihydrogen bonds and halogenâ€“hydride bonds. Comptes Rendus Chimie, 2016, 19, 995-1002.	0.5	3

#	Article	IF	Citations
55	The covalence and infrared spectra of cationic hydrogen bonds and dihydrogen bonds. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450060.	1.8	2
56	AGOA hydration clusters produce the solvation effect on the aziridineÂ·Â·Â·hydrofluoric acid complexÂâ€”ÂA modern proposal. Canadian Journal of Chemistry, 2010, 88, 338-343.	1.1	1
57	The formation of hydride bonds in cationic complexes of nBeH2â€¢â€¢â€¢mX with n=1 or 2, m=1 or 2 and X = Li+ or Na+. Journal of the Serbian Chemical Society, 2014, 79, 1413-1420.	0.8	1
58	The Interaction Strength, Frequency-shifts and Covalence of the C2H4Oâ˜â˜â˜HOCl and C2H5Nâ˜â˜â˜HOCl Heterocyclic Complexes. Orbital, 2017, 9, .	0.3	1
59	Uma nova visÃ£o da tripla hÃ©lice do DNA: parÃ¢metros estruturais, espectroscÃ³picos e eletrÃ´nicos de ligaÃ§Ãµes de hidrogÃªnio para os emparelhamentos de Watson-Crick e Hoogsteen. Semina: CiÃªncias Exatas E TecnolÃ³gicas, 2020, 41, 59.	0.1	1
60	Metodologia AGOA: a modelagem de clusters de hidrataÃ§Ã£o no complexo aziridinaÂ·Â·Â·Ã¡cido fluorÃdrico. Quimica Nova, 2009, 32, 1184-1188.	0.3	0
61	The definitive challenge of forming uncommon pseudoâ€Ï€Â·Â·Â·Hâ€“F and CÂ·Â·Â·Hâ€“F hydrogen bonds on cyclic and cubic nonpolar hydrocarbons. Journal of Physical Organic Chemistry, 2020, 33, e4098.	1.9	0
62	Solvent effect on ternary complexes formed by epoxy and hydrofluoric acid. Journal of the Serbian Chemical Society, 2015, 80, 651-658.	0.8	0
63	QSAR-3D e Docking Molecular de Derivados de Ãcidos N-arilantranÃlicos com Atividade InibitÃ³ria na Enzima Catepsina L. Orbital, 2016, 1, .	0.3	0
64	O paradigma da estrutura do doador de prÃ³ton na formaÃ§Ã£o de ligaÃ§Ãµes de hidrogÃªnio: complexo C2H2â˜â˜â˜6(HF). Quimica Nova, 0, , .	0.3	0