Ibon Alkorta

List of Publications by Citations

931 papers	27,090 citations	69 h-index	125 g-index
992 ext. papers	29,477 ext. citations	3.1 avg, IF	7.6 L-index

#	Paper	IF	Citations
931	From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving XH?FY systems. *Journal of Chemical Physics*, **2002**, 117, 5529-5542	3.8	1196
930	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2	1111
929	Behavior of Ylides Containing N, O, and C Atoms as Hydrogen Bond Acceptors. *Journal of the American Chemical Society*, **2000**, 122, 11154-11161	16	1021
928	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2	738
927	Non-conventional hydrogen bonds. *Chemical Society Reviews*, **1998**, 27, 163	57.5	476
926	Interaction of anions with perfluoro aromatic compounds. *Journal of the American Chemical Society*, **2002**, 124, 8593-8	16	460
925	About the evaluation of the local kinetic, potential and total energy densities in closed-shell interactions. *Chemical Physics Letters*, **2001**, 336, 457-461	2.4	349
924	Relationships between interaction energy, intermolecular distance and electron density properties in hydrogen bonded complexes under external electric fields. *Chemical Physics Letters*, **2011**, 507, 185-189	2.4	255
923	Cooperativity in multiple unusual weak bonds. *Theoretical Chemistry Accounts*, **2010**, 126, 1-14	1.9	242
922	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. *Angewandte Chemie - International Edition*, **2000**, 39, 717-721	16.1	213
921	On the Reliability of Pure and Hybrid DFT Methods for the Evaluation of Halogen, Chalcogen, and Pnicogen Bonds Involving Anionic and Neutral Electron Donors. *Journal of Chemical Theory and Computation*, **2013**, 9, 5201-10	6.2	204
920	Universal features of the electron density distribution in hydrogen-bonding regions: a comprehensive study involving H...X (X=H, C, N, O, F, S, Cl, pi) interactions. *Chemistry - A European Journal*, **2010**, 16, 2442-52	4.6	204
919	Bifurcated Hydrogen Bonds: Three-Centered Interactions. *Journal of Physical Chemistry A*, **1998**, 102, 9925-9932	2.7	198
918	Statistical analysis of (13)C and (15)N NMR chemical shifts from GIAO/B3LYP/6-311 + + G** calculated absolute shieldings. *Magnetic Resonance in Chemistry*, **2007**, 45, 797-800	2	178
917	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. *Journal of Physical Chemistry A*, **1998**, 102, 9278-9285	2.7	175
916	Unusual Hydrogen Bonds: H Interactions. *Journal of Physical Chemistry A*, **1997**, 101, 9457-9463	2.7	173
915	Not Only Hydrogen Bonds: Other Noncovalent Interactions. *Crystals*, **2020**, 10, 180	2.2	169

914	An Attractive Interaction between the π-Cloud of C6F6 and Electron-Donor Atoms. *Journal of Organic Chemistry*, **1997**, 62, 4687-4691	4.1	168
913	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. *Journal of Physical Chemistry A*, **2001**, 105, 743-749	2.7	166
912	Competition of hydrogen bonds and halogen bonds in complexes of hypohalous acids with nitrogenated bases. *Journal of Physical Chemistry A*, **2008**, 112, 10856-63	2.7	159
911	Structures, energies, bonding, and NMR properties of pnicogen complexes H2XP:NXH2 (X ? H, CH3, NH2, OH, F, Cl). *Journal of Physical Chemistry A*, **2011**, 115, 13724-31	2.7	153
910	Theoretical Study of Strong Hydrogen Bonds between Neutral Molecules: The Case of Amine Oxides and Phosphine Oxides as Hydrogen Bond Acceptors. *Journal of Physical Chemistry A*, **1999**, 103, 272-279	2.7	143
909	Beryllium Bonds, Do They Exist?. *Journal of Chemical Theory and Computation*, **2009**, 5, 2763-71	6.2	140
908	Bond Length-Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. *Structural Chemistry*, **1998**, 9, 243-247	1.7	131
907	31P-31P spin-spin coupling constants for pnicogen homodimers. *Chemical Physics Letters*, **2011**, 512, 184-187	2.4	125
906	Pnicogen bonded complexes of PO2X (X = F, Cl) with nitrogen bases. *Journal of Physical Chemistry A* , **2013**, 117, 10497-503	2.7	124
905	Molecular polarization potential maps of the nucleic acid bases. *International Journal of Quantum Chemistry*, **1996**, 57, 123-135	2.1	124
904	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. *Molecular Physics*, **2004**, 102, 2563-2574	1.6	119
903	Intramolecular Hydrogen Bonds inortho-Substituted Hydroxybenzenes and in 8-Susbtituted 1-Hydroxynaphthalenes:Can a Methyl Group Be an Acceptor of Hydrogen Bonds?. *Journal of Physical Chemistry A*, **2001**, 105, 10462-10467	2.7	119
902	Comparison of models to correlate electron density at the bond critical point and bond distance. *Computational and Theoretical Chemistry*, **2000**, 496, 131-137		113
901	Basicity of N-H- and N-Methyl-1,2,3-triazoles in the Gas Phase, in Solution, and in the Solid State An Experimental and Theoretical Study. *European Journal of Organic Chemistry*, **2001**, 2001, 3013	3.1	107
900	Experimental measurements and theoretical calculations of the chemical shifts and coupling constants of three azines (benzalazine, acetophenoneazine and cinnamaldazine). *Magnetic Resonance in Chemistry*, **2008**, 46, 859-64	2	106
899	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acid-Base Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 9791-9800	2.7	101
898	Are resonance-assisted hydrogen bonds resonance assisted? A theoretical NMR study. *Chemical Physics Letters*, **2005**, 411, 411-415	2.4	101
897	Influence of Hydrogen Bonds on the P···P Pnicogen Bond. *Journal of Chemical Theory and Computation*, **2012**, 8, 2320-7	6.2	94

896	Intermolecular weak interactions in HTeXH dimers (X=O, S, Se, Te): hydrogen bonds, chalcogen-chalcogen contacts and chiral discrimination. *ChemPhysChem*, **2012**, 13, 496-503	3.1	92
895	Fluorine□fluorine Interactions: NMR and AIM Analysis. *Structural Chemistry*, **2004**, 15, 117-120	1.7	92
894	Inverse Hydrogen-Bonded Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 4236-4244	2.7	91
893	Pnicogen-bonded cyclic trimers (PH2X)3 with X = F, Cl, OH, NC, CN, CH3, H, and BH2. *Journal of Physical Chemistry A*, **2013**, 117, 4981-7	2.7	89
892	Cooperativity in Tetrel Bonds. *Journal of Physical Chemistry A*, **2016**, 120, 648-56	2.7	88
891	A new avenue to the synthesis of highly substituted pyrroles: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 18619-18631	3.6	88
890	Synthesis, characterization, molecular structure and theoretical studies of axially fluoro-substituted subazaporphyrins. *Chemistry - A European Journal*, **2008**, 14, 1342-50	4.6	86
889	Interplay of F-H□□F hydrogen bonds and P□□N pnicogen bonds. *Journal of Physical Chemistry A*, **2012**, 116, 9205-13	2.7	85
888	Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. *Journal of Physical Chemistry A*, **2002**, 106, 9325-9330	2.7	85
887	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. *Acta Crystallographica Section B: Structural Science*, **2000**, 56 (Pt 6), 1018-28		85
886	Dihydrogen bonds (A□H?H□B). *Chemical Communications*, **1996**, 1633-1634	5.7	84
885	Electrostatics at the origin of the stability of phosphate-phosphate complexes locked by hydrogen bonds. *ChemPhysChem*, **2012**, 13, 1421-4	3.1	81
884	Theoretical study of dihydrogen bonds between (XH)2, X = Li, Na, BeH, and MgH, and weak hydrogen bond donors (HCN, HNC, and HCCH). *Journal of Physical Chemistry A*, **2006**, 110, 10279-86	2.7	80
883	The paradox of hydrogen-bonded anion-anion aggregates in oxoanions: a fundamental electrostatic problem explained in terms of electrophilic□□nucleophilic interactions. *Journal of Physical Chemistry A*, **2015**, 119, 183-94	2.7	79
882	A solid-state NMR, X-ray diffraction, and ab initio computational study of hydrogen-bond structure and dynamics of pyrazole-4-carboxylic acid chains. *Journal of the American Chemical Society*, **2001**, 123, 7898-906	16	79
881	Single electron pnicogen bonded complexes. *Journal of Physical Chemistry A*, **2014**, 118, 947-53	2.7	78
880	Exploring (NH2F)2, H2FP:NFH2, and (PH2F)2 potential surfaces: hydrogen bonds or pnicogen bonds?. *Journal of Physical Chemistry A*, **2013**, 117, 183-91	2.7	78
879	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. *Advances in Heterocyclic Chemistry*, **2012**, 1-188	2.4	78

878	Competition and interplay between hole and 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, 5199-206	2.7	78
877	Ab Initio (GIAO) Calculations of Absolute Nuclear Shieldings for Representative Compounds Containing 1(2)H, 6(7)Li, 11B, 13C, 14(15)N, 17O, 19F, 29Si, 31P, 33S, and 35Cl Nuclei. *Structural Chemistry*, **1998**, 9, 187-202	1.7	78
876	Do traditional, chlorine-shared, and ion-pair halogen bonds exist? An ab initio investigation of FCl:CNX complexes. *Journal of Physical Chemistry A*, **2010**, 114, 12958-62	2.7	77
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873	Theoretical study of the HXYH dimers (X, Y = O, S, Se). Hydrogen bonding and chalcogen halcogen interactions. *Molecular Physics*, **2011**, 109, 2543-2552	1.6	75
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871	Pnicogen bonds between X?PH3 (X = O, S, NH, CH2) and phosphorus and nitrogen bases. *Journal of Physical Chemistry A*, **2014**, 118, 1527-37	2.7	73
870	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. *Journal of Chemical Theory and Computation*, **2012**, 8, 2293-300	6.2	73
869	Open bis(triazolium) structural motifs as a benchmark to study combined hydrogen- and halogen-bonding interactions in oxoanion recognition processes. *Journal of Organic Chemistry*, **2014**, 79, 6959-69	4.1	72
868	Cooperative and diminutive unusual weak bonding in F3CX HMgH Y and F3CX Y HMgH trimers (X = Cl, Br; Y = HCN, and HNC). *Journal of Physical Chemistry A*, **2010**, 114, 12106-11	2.7	72
867	GIAO Calculations of Chemical Shifts in Heterocyclic Compounds. *Structural Chemistry*, **2003**, 14, 377-389	1.7	71
866	Spodium Bonds: Noncovalent Interactions Involving Group 12 Elements. *Angewandte Chemie - International Edition*, **2020**, 59, 17482-17487	16.1	70
865	Orthogonal interactions between nitryl derivatives and electron donors: pnictogen bonds. *Physical Chemistry Chemical Physics*, **2013**, 15, 14310-8	3.5	69
864	Substituent effects on the cooperativity of halogen bonding. *Journal of Physical Chemistry A*, **2013**, 117, 5551-7	2.7	69
863	Review on DFT and ab initio Calculations of Scalar Coupling Constants. *International Journal of Molecular Sciences*, **2003**, 4, 64-92	6.1	69
862	Pnicogen and hydrogen bonds: complexes between PH3X(+) and PH2X systems. *Physical Chemistry Chemical Physics*, **2015**, 17, 3261-72	3.5	68
861	How to determine whether intramolecular H...H interactions can be classified as dihydrogen bonds. *Journal of Physical Chemistry A*, **2008**, 112, 2721-7	2.7	68

860	A review with comprehensive data on experimental indirect scalar NMR spin-spin coupling constants across hydrogen bonds. *Magnetic Resonance in Chemistry*, **2008**, 46, 599-624	2	68
859	Study of the reaction of chalcone analogs of dehydroacetic acid and o-aminothiophenol: synthesis and structure of 1,5-benzothiazepines and 1,4-benzothiazines. *Tetrahedron*, **2005**, 61, 6642-6651	2.3	68
858	Influence of substituent effects on the formation of P□□Cl pnicogen bonds or halogen bonds. *Journal of Physical Chemistry A*, **2014**, 118, 2360-6	2.7	67
857	Discovery of 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-3-hexyl-1h-1,2,4-triazole, a novel in vivo cannabinoid antagonist containing a 1,2,4-triazole motif. *Journal of Medicinal Chemistry*, **2004**, 47, 2939-42	7.9	67
856	Effects of fluorine substitution on hydrogen bond interactions. *Journal of Fluorine Chemistry*, **2000**, 101, 233-238	2.1	67
855	Ab initio hybrid DFT□GIAO calculations of the shielding produced by carbon□arbon bonds and aromatic rings in 1H NMR spectroscopy. *New Journal of Chemistry*, **1998**, 22, 381-385	3.5	67
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853	New page to access pyridine derivatives: synthesis from N-propargylamines. *RSC Advances*, **2016**, 6, 71662-71675	3.6	66
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850	A computational study of the cooperativity in clusters of interhalogen derivatives. *Structural Chemistry*, **2009**, 20, 63-71	1.7	66
849	Novel routes to quinoline derivatives from N-propargylamines. *RSC Advances*, **2016**, 6, 49730-49746	3.6	66
848	Properties of complexes H2C?(X)P:PXH2, for X = F, Cl, OH, CN, NC, CCH, H, CH3, and BH2: P□□P pnicogen bonding at □holes and □holes. *Journal of Physical Chemistry A*, **2013**, 117, 11592-604	2.7	65
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845	Phosphorus as a simultaneous electron-pair acceptor in intermolecular P□□N pnicogen bonds and electron-pair donor to Lewis acids. *Journal of Physical Chemistry A*, **2013**, 117, 3133-41	2.7	63
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842	Discrimination of hydrogen-bonded complexes with axial chirality. *Journal of Chemical Physics*, **2002**, 117, 6463-6468	3.8	62
841	N-Propargylic β-enaminocarbonyls: powerful and versatile building blocks in organic synthesis. *RSC Advances*, **2017**, 7, 13198-13211	3.6	61
840	Carbon...carbon weak interactions. *Journal of Physical Chemistry A*, **2009**, 113, 8387-93	2.7	61
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837	A study of the tautomerism of β-dicarbonyl compounds with special emphasis on curcuminoids. *Tetrahedron*, **2008**, 64, 8089-8094	2.3	58
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817	The Pnicogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnicogen Bonds. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 191-263	0.7	50
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814	A GIAO/DFT study of 1H, 13C and 15N shieldings in amines and its relevance in conformational analysis. *Magnetic Resonance in Chemistry*, **2004**, 42, 955-61	2	50
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797	Recent advances in sulfur–nitrogen bond formation cross-dehydrogenative coupling reactions.. *RSC Advances*, **2018**, 8, 18456-18469	3.6	45
796	Borophene as an electronic sensor for metronidazole drug: A computational study. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107539	2.8	44
795	Complexes between dihydrogen and amine, phosphine, and arsine derivatives. Hydrogen bond versus pnictogen interaction. *Journal of Physical Chemistry A*, **2013**, 117, 3243-51	2.7	44
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789	Radicals as hydrogen bond acceptors. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 429-435		43

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787	3-(2-Pyridyl)-[1,2,3]triazolo[1,5-a]pyridines. An experimental and theoretical (DFT) study of the ring-chain isomerization. *Organic and Biomolecular Chemistry*, **2005**, 3, 3905-10	3.8	43
786	An experimental (NMR) and theoretical (GIAO) study of the tautomerism of benzotriazole in solution. *Tetrahedron*, **2002**, 58, 9089-9094	2.3	43
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784	Properties of Cationic Pnicogen-Bonded Complexes F(4-n)H(n)P(+):N-Base with F-P□□N Linear and n = 0-3. *Journal of Physical Chemistry A*, **2015**, 119, 5853-64	2.7	42
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