Ibon Alkorta

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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	3.9	1196
930	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	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	16.4	1021
928	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
927	Non-conventional hydrogen bonds. *Chemical Society Reviews*, **1998**, 27, 163	58.5	476
926	Interaction of anions with perfluoro aromatic compounds. *Journal of the American Chemical Society*, **2002**, 124, 8593-8	16.4	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	2.5	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	2.5	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	16.4	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	6.4	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	4.8	204
919	Bifurcated Hydrogen Bonds: Three-Centered Interactions. *Journal of Physical Chemistry A*, **1998**, 102, 9925-9932	2.8	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	2.1	178
917	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. *Journal of Physical Chemistry A*, **1998**, 102, 9278-9285	2.8	175
916	Unusual Hydrogen Bonds: H Interactions. *Journal of Physical Chemistry A*, **1997**, 101, 9457-9463	2.8	173
915	Not Only Hydrogen Bonds: Other Noncovalent Interactions. *Crystals*, **2020**, 10, 180	2.3	169

914	An Attractive Interaction between the π-Cloud of C6F6 and Electron-Donor Atoms. *Journal of Organic Chemistry*, **1997**, 62, 4687-4691	4.2	168
913	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. *Journal of Physical Chemistry A*, **2001**, 105, 743-749	2.8	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	2.8	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	2.8	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	2.8	143
909	Beryllium Bonds, Do They Exist?. *Journal of Chemical Theory and Computation*, **2009**, 5, 2763-71	6.4	140
908	Bond Length-Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. *Structural Chemistry*, **1998**, 9, 243-247	1.8	131
907	31P-31P spin-spin coupling constants for pnicogen homodimers. *Chemical Physics Letters*, **2011**, 512, 184-187	2.5	125
906	Pnicogen bonded complexes of PO2X (X = F, Cl) with nitrogen bases. *Journal of Physical Chemistry A* , **2013**, 117, 10497-503	2.8	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	1.7	119
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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	3.2	107
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899	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acid-Base Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 9791-9800	2.8	101
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897	Influence of Hydrogen Bonds on the P···P Pnicogen Bond. *Journal of Chemical Theory and Computation*, **2012**, 8, 2320-7	6.4	94

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895	Fluorine□fluorine Interactions: NMR and AIM Analysis. *Structural Chemistry*, **2004**, 15, 117-120	1.8	92
894	Inverse Hydrogen-Bonded Complexes. *Journal of Physical Chemistry A*, **1997**, 101, 4236-4244	2.8	91
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892	Cooperativity in Tetrel Bonds. *Journal of Physical Chemistry A*, **2016**, 120, 648-56	2.8	88
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890	Synthesis, characterization, molecular structure and theoretical studies of axially fluoro-substituted subazaporphyrins. *Chemistry - A European Journal*, **2008**, 14, 1342-50	4.8	86
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881	Single electron pnicogen bonded complexes. *Journal of Physical Chemistry A*, **2014**, 118, 947-53	2.8	78
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879	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. *Advances in Heterocyclic Chemistry*, **2012**, 1-188	2.4	78

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