Jose Elguero

List of Publications by Year
in descending order

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1,182 papers	35,959 citations	6592 79 h-index	13338 130 g-index
1204 all docs	1204 docs citations	1204 times ranked	16605 citing authors

#	Article	IF	Citations
1	From weak to strong interactions: A comprehensive analysis of the topological and energetic properties of the electron density distribution involving Xâ€“Hâ‹¯Fâ€“Y systems. Journal of Chemical Physics, 2002, 117, 5529-5542.	1.2	1,510
2	Behavior of Ylides Containing N, O, and C Atoms as Hydrogen Bond Acceptors. Journal of the American Chemical Society, 2000, 122, 11154-11161.	6.6	1,334
3	Non-conventional hydrogen bonds. Chemical Society Reviews, 1998, 27, 163.	18.7	564
4	Interaction of Anions with Perfluoro Aromatic Compounds. Journal of the American Chemical Society, 2002, 124, 8593-8598.	6.6	496
5	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	1.0	289
6	The Tautomerism of Heterocycles: Five-membered Rings with Two or More Heteroatoms. Advances in Heterocyclic Chemistry, 2000, 76, 157-323.	0.9	268
7	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	0.5	254
8	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, 5201-5210.	2.3	243
9	Water Clusters: Towards an Understanding Based on First Principles of Their Static and Dynamic Properties. Angewandte Chemie - International Edition, 2000, 39, 717-721.	7.2	229
10	Bifurcated Hydrogen Bonds:â€‰ Three-Centered Interactions. Journal of Physical Chemistry A, 1998, 102, 9925-9932.	1.1	225
11	Photoinduced intramolecular proton transfer as the mechanism of ultraviolet stabilizers: a reappraisal. Journal of the American Chemical Society, 1990, 112, 747-759.	6.6	198
12	Nâ€polyazolylmethanes. 1. Synthesis and nmr study of N,Nâ€²â€diazolylmethanes. Journal of Heterocyclic Chemistry, 1982, 19, 1141-1145.	1.4	194
13	Carbon-13 magnetic resonance studies of azoles. Tautomerism, shift reagent effects, and solvent effects. Journal of Organic Chemistry, 1974, 39, 357-363.	1.7	191
14	Basicity and Acidity of Azoles. Advances in Heterocyclic Chemistry, 1987, , 187-274.	0.9	187
15	Charge-Transfer Complexes between Dihalogen Compounds and Electron Donors. Journal of Physical Chemistry A, 1998, 102, 9278-9285.	1.1	187
16	Statistical analysis of ¹³C and ¹⁵N NMR chemical shifts from GIAO/B3LYP/6â€311 + + G** calculated absolute shieldings. Magnetic Resonance in Chemistry, 2007, 45, 797-800.	1.1	186
17	Molecular Complexes between Silicon Derivatives and Electron-Rich Groups. Journal of Physical Chemistry A, 2001, 105, 743-749.	1.1	182
18	Unusual Hydrogen Bonds:Â HÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 1997, 101, 9457-9463.	1.1	180

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19	An Attractive Interaction between the Ï€-Cloud of C6F6 and Electron-Donor Atoms. Journal of Organic Chemistry, 1997, 62, 4687-4691.	1.7	176
20	Competition of Hydrogen Bonds and Halogen Bonds in Complexes of Hypohalous Acids with Nitrogenated Bases. Journal of Physical Chemistry A, 2008, 112, 10856-10863.	1.1	170
21	Structures, Energies, Bonding, and NMR Properties of Pnicogen Complexes H₂XP:NXH₂(X â••H, CH₃, NH₂, OH, F, Cl). Journal of Physical Chemistry A, 2011, 115, 13724-13731.	1.1	170
22	Beryllium Bonds, Do They Exist?. Journal of Chemical Theory and Computation, 2009, 5, 2763-2771.	2.3	158
23	Effect ofN-substituents on the13C NMR parameters of azoles. Magnetic Resonance in Chemistry, 1988, 26, 134-151.	1.1	154
24	Theoretical Study of Strong Hydrogen Bonds between Neutral Molecules:â€‰ The Case of Amine Oxides and Phosphine Oxides as Hydrogen Bond Acceptors. Journal of Physical Chemistry A, 1999, 103, 272-279.	1.1	154
25	Prototropic Tautomerism of Heterocycles: Heteroaromatic Tautomerismâ€”General Overview and Methodology. Advances in Heterocyclic Chemistry, 2000, 76, 1-84.	0.9	154
26	IMPROVED SYNTHESIS OF POLYAZOLYLMETHANES UNDER SOLID-LIQUID PHASE-TRANSFER CATALYSIS. Organic Preparations and Procedures International, 1984, 16, 299-307.	0.6	146
27	Bond Lengthâ€“Electron Density Relationships: From Covalent Bonds to Hydrogen Bond Interactions. Structural Chemistry, 1998, 9, 243-247.	1.0	143
28	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
29	New ultraviolet stabilizers: 3- and 5-(2'-hydroxyphenyl)pyrazoles. Journal of the American Chemical Society, 1992, 114, 5039-5048.	6.6	139
30	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	7.2	136
31	Pyrazoles. , 1996, , 1-75.		135
32	31Pâ€“31P spinâ€“spin coupling constants for pnicogen homodimers. Chemical Physics Letters, 2011, 512, 184-187.	1.2	132
33	Pnicogen Bonded Complexes of PO₂X (X = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2013, 117, 10497-10503.	1.1	129
34	Basicity and acidity of azoles: the annelation effect in azoles. Journal of the American Chemical Society, 1988, 110, 4105-4111.	6.6	127
35	Intramolecular Hydrogen Bonds inortho-Substituted Hydroxybenzenes and in 8-Susbtituted 1-Hydroxynaphthalenes:Â Can a Methyl Group Be an Acceptor of Hydrogen Bonds?. Journal of Physical Chemistry A, 2001, 105, 10462-10467.	1.1	126
36	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. Molecular Physics, 2004, 102, 2563-2574.	0.8	126

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37	Intermolecular triple proton and deuteron transfer in crystalline 3,5-dimethylpyrazole studied by NMR, NQR, and x-ray methods. Journal of the American Chemical Society, 1989, 111, 7304-7312.	6.6	123
38	13C NMR of pyrazoles. Magnetic Resonance in Chemistry, 1993, 31, 107-168.	1.1	123
39	Basicity of N-H- and N-Methyl-1,2,3-triazoles in the Gas Phase, in Solution, and in the Solid State â˜† An Experimental and Theoretical Study. European Journal of Organic Chemistry, 2001, 2001, 3013.	1.2	121
40	Electrostatic proximity effects in the relative basicities and acidities of pyrazole, imidazole, pyridazine, and pyrimidine. Journal of the American Chemical Society, 1986, 108, 3237-3239.	6.6	120
41	Tautomerism and aromaticity in 1,2,3-triazoles: the case of benzotriazole. Journal of the American Chemical Society, 1989, 111, 7348-7353.	6.6	119
42	Theoretical Study of the Influence of Electric Fields on Hydrogen-Bonded Acidâ˜Base Complexes. Journal of Physical Chemistry A, 1997, 101, 9791-9800.	1.1	114
43	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, 859-864.	1.1	109
44	Observation of a series of degenerate cyclic double, triple, and quadruple proton transfers in solid pyrazoles. Journal of the American Chemical Society, 1992, 114, 9657-9659.	6.6	107
45	Are resonance-assisted hydrogen bonds â€˜resonance assistedâ€™? A theoretical NMR study. Chemical Physics Letters, 2005, 411, 411-415.	1.2	106
46	Influence of Hydrogen Bonds on the PÂ·Â·Â·P Pnicogen Bond. Journal of Chemical Theory and Computation, 2012, 8, 2320-2327.	2.3	106
47	Fluorescence of fullerenes (C60 and C70). Journal of the American Chemical Society, 1993, 115, 9249-9252.	6.6	105
48	Fluorineâ€“Fluorine Interactions: NMR and AIM Analysis. Structural Chemistry, 2004, 15, 117-120.	1.0	103
49	Cooperativity in Tetrel Bonds. Journal of Physical Chemistry A, 2016, 120, 648-656.	1.1	103
50	Intermolecular Weak Interactions in HTeXH Dimers (X=O, S, Se, Te): Hydrogen Bonds, Chalcogenâ€“Chalcogen Contacts and Chiral Discrimination. ChemPhysChem, 2012, 13, 496-503.	1.0	101
51	Very strong hydrogen bonds in neutral molecules: The phosphinic acid dimers. Journal of Chemical Physics, 1998, 109, 2685-2693.	1.2	100
52	Current TrÃ¶ger's Base Chemistry. Advances in Heterocyclic Chemistry, 2007, 93, 1-56.	0.9	98
53	Substituent effects on the15N NMR Parameters of Azoles. , 1997, 35, 35-75.		96
54	Inverse Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 1997, 101, 4236-4244.	1.1	95

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55	Dynamic NMR Study of the Mechanisms of Double, Triple, and Quadruple Proton and Deuteron Transfer in Cyclic Hydrogen Bonded Solids of Pyrazole Derivatives. Journal of the American Chemical Society, 2004, 126, 11718-11732.	6.6	95
56	Dihydrogen bonds (Aâ€“Hâ‹¯Hâ€“B). Chemical Communications, 1996, , 1633-1634.	2.2	94
57	Pnicogen-Bonded Cyclic Trimers (PH₂X)₃ with X = F, Cl, OH, NC, CN, CH₃, H, and BH₂. Journal of Physical Chemistry A, 2013, 117, 4981-4987.	1.1	94
58	Supramolecular structure of 1H-pyrazoles in the solid state: a crystallographic and ab initio study. Acta Crystallographica Section B: Structural Science, 2000, 56, 1018-1028.	1.8	93
59	Synthesis, Characterization, Molecular Structure and Theoretical Studies of Axially Fluoroâ€Substituted Subazaporphyrins. Chemistry - A European Journal, 2008, 14, 1342-1350.	1.7	93
60	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.	1.1	90
61	Interplay of Fâ€“H^{...}F Hydrogen Bonds and P^{...}N Pnicogen Bonds. Journal of Physical Chemistry A, 2012, 116, 9205-9213.	1.1	90
62	The geometry of pyrazole: A test forab initiocalculations. Journal of Computational Chemistry, 1995, 16, 263-272.	1.5	89
63	Title is missing!. Structural Chemistry, 1998, 9, 187-202.	1.0	89
64	Dynamic intermolecular tautomerism of 3,5-dimethylpyrazole in the solid state by carbon-13 CP/MAS NMR spectroscopy and x-ray crystallography. Journal of the American Chemical Society, 1985, 107, 5290-5291.	6.6	87
65	Self-Discrimination of Enantiomers in Hydrogen-Bonded Dimers. Journal of the American Chemical Society, 2002, 124, 1488-1493.	6.6	86
66	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.	1.1	86
67	Theoretical study of the azido-tetrazole isomerization. Journal of the American Chemical Society, 1976, 98, 1685-1690.	6.6	85
68	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, 10279-10286.	1.1	85
69	Carbenes and Silylenes as Hydrogen Bond Acceptors. The Journal of Physical Chemistry, 1996, 100, 19367-19370.	2.9	84
70	Atropisomerism and Axial Chirality in Heteroaromatic Compounds. Advances in Heterocyclic Chemistry, 2012, , 1-188.	0.9	84
71	Single Electron Pnicogen Bonded Complexes. Journal of Physical Chemistry A, 2014, 118, 947-953.	1.1	84
72	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, 7898-7906.	6.6	83

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73	New Chiral Molecular Tweezers with a Bis-TrÃ¶ger's Base Skeletonâ€. Journal of Organic Chemistry, 2001, 66, 1607-1611.	1.7	82
74	Substituent and solvent effects on the proton transfer equilibrium in anils and azo derivatives of naphthol. Multinuclear NMR study and theoretical calculations. Journal of Molecular Structure, 2004, 705, 1-9.	1.8	82
75	Nonâ€Resonanceâ€Assisted Hydrogen Bonding in Hydroxymethylene and Aminomethylene Cyclobutanones and Cyclobutenones and Their Nitrogen Counterparts.. ChemPhysChem, 2007, 8, 1950-1958.	1.0	82
76	A 13C NMR spectroscopy study of the structure of N-H pyrazoles and indazoles. Canadian Journal of Chemistry, 1993, 71, 678-684.	0.6	81
77	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, 12958-12962.	1.1	81
78	Modulating the Strength of Hydrogen Bonds through Beryllium Bonds. Journal of Chemical Theory and Computation, 2012, 8, 2293-2300.	2.3	81
79	Exploring (NH₂F)₂, H₂FP:NFH₂, and (PH₂F)₂ Potential Surfaces: Hydrogen Bonds or Pnicogen Bonds?. Journal of Physical Chemistry A, 2013, 117, 183-191.	1.1	81
80	Effects of Nitrogen Substitution in Poly(Pyrazolyl)Borato Ligands: From Orbital Energy Levels to Câ€“H âƒ› O Hydrogen Bonding. Chemistry - A European Journal, 1996, 2, 992-1000.	1.7	80
81	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
82	Theoretical study of the HXYH dimers (X,â€‰Yâ€‰=â€‰O, S, Se). Hydrogen bonding and chalcogenâ€“chalcogen interactions. Molecular Physics, 2011, 109, 2543-2552.	0.8	80
83	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, 6959-6969.	1.7	80
84	Structures, Binding Energies, and Spinâ€“Spin Coupling Constants of Geometric Isomers of Pnicogen Homodimers (PHFX)₂, X = F, Cl, CN, CH₃, NC. Journal of Physical Chemistry A, 2012, 116, 3056-3060.	1.1	79
85	Title is missing!. Helvetica Chimica Acta, 2002, 85, 2763-2776.	1.0	78
86	Review on DFT and ab initio Calculations of Scalar Coupling Constants. International Journal of Molecular Sciences, 2003, 4, 64-92.	1.8	78
87	A review with comprehensive data on experimental indirect scalar NMR spinâ€“spin coupling constants across hydrogen bonds. Magnetic Resonance in Chemistry, 2008, 46, 599-624.	1.1	78
88	The reaction between hydrazines and Î²-dicarbonyl compounds: proposal for a mechanism. Canadian Journal of Chemistry, 2000, 78, 1109-1120.	0.6	77
89	How To Determine Whether Intramolecular HÂ·Â·Â·H Interactions Can Be Classified as Dihydrogen Bonds. Journal of Physical Chemistry A, 2008, 112, 2721-2727.	1.1	77
90	Pnicogen Bonds between Xâ•PH₃ (X = O, S, NH, CH₂) and Phosphorus and Nitrogen Bases. Journal of Physical Chemistry A, 2014, 118, 1527-1537.	1.1	77

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91	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.	1.0	76
92	Orthogonal interactions between nitryl derivatives and electron donors: pnictogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 14310.	1.3	75
93	Influence of Substituent Effects on the Formation of PÂ·Â·Â·Cl Pnicogen Bonds or Halogen Bonds. Journal of Physical Chemistry A, 2014, 118, 2360-2366.	1.1	75
94	Azolides. Part 12. Carbon-13 nuclear magnetic resonance study of N-methyl and N-acetyl derivatives of azoles and benzazoles. Journal of the Chemical Society Perkin Transactions II, 1978, , 99.	0.9	74
95	GIAO Calculations of Chemical Shifts in Heterocyclic Compounds. Structural Chemistry, 2003, 14, 377-389.	1.0	74
96	Pnicogen and hydrogen bonds: complexes between PH3X+ and PH2X systems. Physical Chemistry Chemical Physics, 2015, 17, 3261-3272.	1.3	74
97	Effects of fluorine substitution on hydrogen bond interactions. Journal of Fluorine Chemistry, 2000, 101, 233-238.	0.9	73
98	CarbonÂ·Â·Â·Carbon Weak Interactions. Journal of Physical Chemistry A, 2009, 113, 8387-8393.	1.1	73
99	A computational study of the cooperativity in clusters of interhalogen derivatives. Structural Chemistry, 2009, 20, 63-71.	1.0	70
100	Influence of Lone Pair Repulsion vs Resonance Energy on the Relative Stabilities of Molecular Structures: A Theoretical Approach to the Equilibrium between 1H- and 2H-Benzotriazole Tautomers. Journal of Organic Chemistry, 1994, 59, 2799-2802.	1.7	69
101	Polymorphism and Desmotropy in Heterocyclic Crystal Structures. Crystal Growth and Design, 2011, 11, 4731-4738.	1.4	69
102	Acidity and Basicity of Indazole and its N-Methyl Derivatives in the Ground and in the Excited State. The Journal of Physical Chemistry, 1994, 98, 10606-10612.	2.9	68
103	Field effects on dihydrogen bonded systems. Chemical Physics Letters, 1997, 275, 423-428.	1.2	68
104	Pnicogen-Bonded Anionic Complexes. Journal of Physical Chemistry A, 2014, 118, 3386-3392.	1.1	68
105	Large Chiral Recognition in Hydrogen-Bonded Complexes and Proton Transfer in Pyrrolo[2,3-b]pyrrole Dimers as Model Compounds. Journal of Organic Chemistry, 2003, 68, 7485-7489.	1.7	67
106	Periodic Trends in Bond Dissociation Energies. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 4359-4365.	1.1	67
107	Properties of Complexes H₂Câ•(X)P:PXH₂, for X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂: PÂ·Â·Â·P Pnicogen Bonding at Ïƒ-Holes and Ï€-Holes. Journal of Physical Chemistry A, 2013, 117, 11592-11604.	1.1	67
108	Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular PÂ·Â·Â·N Pnicogen Bonds and Electron-Pair Donor to Lewis Acids. Journal of Physical Chemistry A, 2013, 117, 3133-3141.	1.1	66

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109	Orientation de la rÃ©action d'alkylation des pyrazoles dans des conditions neutres et en catalyse par transfert de phase. Journal of Heterocyclic Chemistry, 1980, 17, 137-142.	1.4	65
110	A study of the tautomerism of Î²-dicarbonyl compounds with special emphasis on curcuminoids. Tetrahedron, 2008, 64, 8089-8094.	1.0	65
111	Characterizing Complexes with Pnicogen Bonds Involving sp² Hybridized Phosphorus Atoms: (H₂Câ•PX)₂ with X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂. Journal of Physical Chemistry A, 2013, 117, 6893-6903.	1.1	65
112	Self-assembly of Ligands Designed for the Building of a New Type of [2 Ã— 2] Metallic Grid. Anion Encapsulation and Diffusion NMR Spectroscopy. Inorganic Chemistry, 2008, 47, 413-428.	1.9	64
113	The tautomerism of 3(5)-phenylpyrazoles: an experimental (1H, 13C, 15N NMR and X-ray crystallography) study. Journal of the Chemical Society Perkin Transactions II, 1992, , 1737.	0.9	63
114	Enthalpies of Formation ofN-Substituted Pyrazoles and Imidazoles. Journal of Physical Chemistry A, 1999, 103, 9336-9344.	1.1	63
115	Discrimination of hydrogen-bonded complexes with axial chirality. Journal of Chemical Physics, 2002, 117, 6463-6468.	1.2	63
116	Influence of Intermolecular Hydrogen Bonds on the Tautomerism of Pyridine Derivatives. Journal of Organic Chemistry, 2002, 67, 1515-1519.	1.7	63
117	A theoretical study of the tautomerism and ionization of 5-substituted NH-tetrazoles. Computational and Theoretical Chemistry, 2004, 668, 123-132.	1.5	63
118	On the Existence of Î±-Agostic Bonds:â€‰ Bonding Analyses of Titanium Alkyl Complexes. Organometallics, 2006, 25, 5638-5647.	1.1	63
119	Structure of bis-, tris- and tetrakispyrazolylborates in the solid state (sodium and potassium salts of) Tj ETQq1 1 0.784314 rgBT /Overlock Chimica Acta, 1990, 176, 195-204.	1.2	60
120	THE CHEMISTRY OF PYRAZOLIDINONES. A REVIEW. Organic Preparations and Procedures International, 1991, 23, 273-320.	0.6	60
121	The structure of halogeno-1,2,4-triazoles in the solid state and in solution. New Journal of Chemistry, 2001, 25, 1061-1068.	1.4	60
122	New Bis(chalcones) and Their Transformation into Bis(pyrazoline) and Bis(pyrazole) Derivatives. European Journal of Organic Chemistry, 2003, 2003, 747-755.	1.2	60
123	Intramolecular pnicogen interactions in phosphorus and arsenic analogues of proton sponges. Physical Chemistry Chemical Physics, 2014, 16, 15900-15909.	1.3	60
124	Atropisomerism and conformational aspects of meso-tetraarylporphyrins and related compounds. Journal of Porphyrins and Phthalocyanines, 2011, 15, 1-28.	0.4	59
125	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.	0.6	59
126	Experimental and theoretical study of the R3P+-X- bond. Case of betaines derived from N-iminophosphoranes and alkyl isocyanates. Journal of the American Chemical Society, 1989, 111, 355-363.	6.6	58

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127	Synthesis and molecular structure of 3-(2-benzyloxy-6-hydroxyphenyl)-5-styrylpyrazoles. Reaction of 2-styrylchromones and hydrazine hydrate. Tetrahedron, 1999, 55, 10187-10200.	1.0	58
128	The tautomerism of Omeprazole in solution: a1H and13C NMR study. Magnetic Resonance in Chemistry, 2004, 42, 712-714.	1.1	58
129	The Structure of Pyrazoles in the Solid State:Â A Combined CPMAS, NMR, and Crystallographic Study. Journal of Organic Chemistry, 2006, 71, 6881-6891.	1.7	58
130	Homo- and heterochiral dimers (PHFX)2, X=Cl, CN, CH3, NC: To what extent do they differ?. Chemical Physics Letters, 2012, 538, 14-18.	1.2	58
131	Hydrogen Bond vs Proton Transfer between Neutral Molecules in the Gas Phase. Journal of Physical Chemistry A, 2001, 105, 7481-7485.	1.1	57
132	Green synthesis and self-association of 2,4-diamino-1,3,5-triazine derivatives. New Journal of Chemistry, 2004, 28, 952-958.	1.4	57
133	The azido-tetrazole and diazo-1,2,3-triazole tautomerism in six-membered heteroaromatic rings and their relationships with aromaticity: Azines and perimidine. Tetrahedron, 2010, 66, 2863-2868.	1.0	57
134	Nâ€polylazolylmÃ©thanes. III.. SynthÃ¨se et Ã©tude rmn du proton des dÃ©rivÃ©s du mÃ©thylÃ¨neâ€1,1â€² diimidazole et du mÃ©thylÃ¨neâ€1,1â€² dibenzimidazole. Journal of Heterocyclic Chemistry, 1983, 20, 1245-1249.	1.4	56
135	Tautomerism and acidity in 4-quinolone-3-carboxylic acid derivatives. Tetrahedron, 1992, 48, 6135-6150.	1.0	56
136	Theoretical estimation of the annular tautomerism of indazoles. Journal of Physical Organic Chemistry, 2005, 18, 719-724.	0.9	56
137	Tris(pyrazol-1-yl)methane-rhodium(I) and -iridium(I) complexes; cyrstal structure of [Rh(COD)(tpzm)][RhCl2(COD)]Â·3CHCl3. Journal of Organometallic Chemistry, 1988, 344, 93-108.	0.8	55
138	New synthetic approaches to condensed pyridazinones: alkylpyridazinyl carbonitriles as building blocks for the synthesis of condensed pyridazinones. Tetrahedron, 1995, 51, 12745-12762.	1.0	55
139	Importance of aromaticity on the relative stabilities of indazole annular tautomers: an ab initio study. Journal of the Chemical Society Perkin Transactions II, 1996, , 57-60.	0.9	55
140	Theoretical Study of HCN and HNC Neutral and Charged Clusters. Journal of Physical Chemistry B, 2005, 109, 18189-18194.	1.2	55
141	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
142	Carbon-13 NMR studies of nitrogen compounds. Iâ€"substituent effects of amino, acetamido, diacetamido, ammonium and trimethylammonium groups. Magnetic Resonance in Chemistry, 1980, 14, 20-24.	0.7	54
143	Interpreting2hJ(F,N),1hJ(H,N) and1J(F,H) in the hydrogen-bonded FH-collidine complex. Magnetic Resonance in Chemistry, 2002, 40, 767-771.	1.1	54
144	13C NMR chemical shifts ofN-unsubstituted- andN-methyl-pyrazole derivatives. Magnetic Resonance in Chemistry, 1984, 22, 603-607.	0.7	53

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145	Complete energy profile of a chiral propeller compound: Tris-(2â€²-methylbenzimidazol-1â€²-yl) Methane (TMBM). Chromatographic resolution on triacetyl cellulose, x-ray structures of the racemic and one enantiomer, and dynamic NMR study. Tetrahedron: Asymmetry, 1990, 1, 65-86.	1.8	53
146	1,2-Proton shifts in pyrazole and related systems: a computational study of [1,5]-sigmatropic migrations of hydrogen and related phenomenaâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1998, , 2497-2504.	0.9	53
147	On the Relationship between the Preferred Site of Hydrogen Bonding and Protonation. Journal of Physical Chemistry A, 2005, 109, 5509-5517.	1.1	53
148	Aromatic Systems as Charge Insulators:Â Their Simultaneous Interaction with Anions and Cations. Journal of Physical Chemistry A, 2003, 107, 9428-9433.	1.1	52
149	Interaction Energies and NMR Indirect Nuclear Spinâ^'Spin Coupling Constants in Linear HCN and HNC Complexes. Journal of Physical Chemistry A, 2005, 109, 6555-6564.	1.1	52
150	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. Journal of Chemical Theory and Computation, 2009, 5, 1186-1194.	2.3	52
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