Ibon Alkorta

List of Publications by Year
in descending order

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957 papers	31,716 citations	9264 74 h-index	11308 136 g-index
993 all docs	993 docs citations	993 times ranked	16587 citing authors

#	Article	IF	Citations
1	Dismantlement of ammonia upon interaction with Be<scp>_n</scp>(<scp>n</scp>Âå‰ 10) clusters. Journal of Computational Chemistry, 2023, 44, 159-167.	3.3	3
2	Performance of Silicon Carbide Nanomaterials in Separation Process. Separation and Purification Reviews, 2023, 52, 205-220.	5.5	3
3	Polyhedra, Tiles and Graphene Defects: The Case of Tetraoctite. Mini-Reviews in Organic Chemistry, 2022, 19, 138-145.	1.3	2
4	The effect of the hybrid multi-layered Graphene oxide/Talc as a hydrophobic agent in epoxy coating. Plastics, Rubber and Composites, 2022, 51, 13-34.	2.0	4
5	The interaction between ethionamide and pristine, Si-, Ga-, and Al-doped boron nitride nanoflakes: A computational study. Journal of Sulfur Chemistry, 2022, 43, 78-94.	2.0	3
6	The use of DOSY experiments to determine the solution structures of coinage metal pyrazolates: The case of {[3,5â€(CF₃)₂Pz]Ag}₃. Magnetic Resonance in Chemistry, 2022, 60, 442-451.	1.9	0
7	Self-Assembled Lanthanide Antenna Glutathione Sensor for the Study of Immune Cells. ACS Sensors, 2022, 7, 322-330.	7.8	5
8	A reduced electrophilicity for simple Lewis acids A involved in non-covalent interactions with Lewis bases B. Physical Chemistry Chemical Physics, 2022, 24, 6856-6865.	2.8	4
9	Density functional theory studies on C20 with substitutional TinNn impurities. Journal of Molecular Modeling, 2022, 28, 62.	1.8	4
10	Stand up for Electrostatics: The Disiloxane Case. ChemPhysChem, 2022, 23, .	2.1	3
11	Determination of the tautomerism of albendazole desmotropes using solution and solid state NMR together with DFT theoretical calculations, both energies and chemical shifts. Journal of Molecular Structure, 2022, 1261, 132883.	3.6	3
12	Perfluorination of Aromatic Compounds Reinforce Their van der Waals Interactions with Rare Gases: The Rotational Spectrum of Pentafluoropyridine-Ne. Molecules, 2022, 27, 17.	3.8	3
13	A DFT study of the tautomerism of 1H-benzo[de]cinnolines and their protonated forms. Theoretical Chemistry Accounts, 2022, 141, 1.	1.4	2
14	Study of the Addition Mechanism of 1H-Indazole and Its 4-, 5-, 6-, and 7-Nitro Derivatives to Formaldehyde in Aqueous Hydrochloric Acid Solutions. Journal of Organic Chemistry, 2022, 87, 5866-5881.	3.2	2
15	Strategies for the direct oxidative esterification of thiols with alcohols. RSC Advances, 2022, 12, 14521-14534.	3.6	3
16	Nucleophilicity of the boron atom in compounds R-B, (R = F, Cl, Br, I, CN, NC, CH3, SiH3, CF3, H): a new look at the inductive effects of the groups R. Physical Chemistry Chemical Physics, 2022, , .	2.8	3
17	Theoretical study of the NO₃radical reaction with CH₂ClBr, CH₂ICl, CH₂BrI, CHCl₂Br, and CHClBr₂. Physical Chemistry Chemical Physics, 2022, 24, 14365-14374.	2.8	3
18	Hydro-trifluoromethyl(thiol)ation of alkenes: a review*. Journal of Sulfur Chemistry, 2022, 43, 519-539.	2.0	1

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19	Methods for Direct Reductive N-Methylation of Nitro Compounds. Topics in Current Chemistry, 2022, 380, .	5.8	3
20	Characterizing the nâ†'Ï€* interaction of pyridine with small ketones: a rotational study of pyridineâ‹¯acetone and pyridineâ‹¯2-butanone. Physical Chemistry Chemical Physics, 2022, 24, 15484-15493.	2.8	5
21	Rotational Behavior of N-(5-Substituted-pyrimidin-2-yl)anilines: Relayed Electronic Effect in Two Nâ€“Ar Bond Rotations. Journal of Organic Chemistry, 2022, 87, 8118-8125.	3.2	3
22	Use of 5,10â€Disubstituted Dibenzoazaborines and Dibenzophosphaborines as Cyclic Supports of Frustrated Lewis Pairs for the Capture of CO₂. ChemPhysChem, 2022, 23, .	2.1	6
23	A DFT quest for effects of fused rings on the stability of remote N-heterocyclic carbenes. Structural Chemistry, 2021, 32, 787-798.	2.0	8
24	Multinuclear magnetic resonance studies of five silver(I) trinuclear pyrazolate complexes. Structural Chemistry, 2021, 32, 215-224.	2.0	3
25	A static and dynamic NMR study of 10â€hydrazinoâ€BODIPY. Magnetic Resonance in Chemistry, 2021, 59, 454-464.	1.9	1
26	Computational study of aÂB36 borophene as an electronic sensor for the anti-cancer drug cisplatinum. Journal of Computational Electronics, 2021, 20, 635-642.	2.5	11
27	A structural analysis of 2,5â€diarylâ€4 H â€2,4â€dihydroâ€3 H â€1,2,4â€triazolâ€3â€ones: NMR in the solid state, Xâ€ray crystallography, and GIPAW calculations. Magnetic Resonance in Chemistry, 2021, 59, 423-438.	1.9	4
28	A new strategy for the synthesis of 2-mercaptobenzazole derivatives by green chemistry metrics. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 1-5.	1.6	1
29	Ultrasound Assisted Chromatography-Free Synthesis of Triazolo [1,2-a]Indazole-Triones in the Presence of 1,4-Diazabicyclo[2.2.2] Octanium Diacetate as an Environmentally Friendly Green Media. Polycyclic Aromatic Compounds, 2021, 41, 963-973.	2.6	2
30	Hexa-cata-hexabenzocoronene nanographene as a promising anode material for Mg-ion batteries. Journal of Molecular Modeling, 2021, 27, 45.	1.8	2
31	Intermolecular difunctionalization of alkenes: synthesis of Î²-hydroxy sulfides. RSC Advances, 2021, 11, 13138-13151.	3.6	33
32	Vicinal halo-trifluoromethylation of alkenes. RSC Advances, 2021, 11, 14941-14955.	3.6	28
33	The recent development of donepezil structure-based hybrids as potential multifunctional anti-Alzheimer's agents: highlights from 2010 to 2020. RSC Advances, 2021, 11, 30781-30797.	3.6	24
34	On the 3D â†' 2D Isomerization of Hexaborane(12). Chemistry, 2021, 3, 28-38.	2.2	4
35	Recent trends in the direct oxyphosphorylation of Câ€“C multiple bonds. RSC Advances, 2021, 11, 470-483.	3.6	18
36	Progress and recent trends in the direct selenocyanation of (hetero)aromatic Câ€“H bonds. RSC Advances, 2021, 11, 22305-22316.	3.6	13

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37	Recent progress in application of nanocatalysts for carbonylative Suzuki cross-coupling reactions. RSC Advances, 2021, 11, 2112-2125.	3.6	15
38	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	2.8	3
39	Non-Covalent Interactions of the Lewis Acids Cuâ€“X, Agâ€“X, and Auâ€“X (X = F and Cl) with Nine Simple Lewis Bases B: A Systematic Investigation of Coinageâ€“Metal Bonds by Ab Initio Calculations. Inorganics, 2021, 9, 13.	2.7	8
40	A theoretical study of inversion barriers and NMR chemical shifts of 3â€pyrazolines (2,3 â€dihydroâ€1 H) Tj ETQq0 0 0 rgBT /Overlock 10	2.6	1
41	An efficient one-pot synthesis of novel 6-hydroxy-14-aryl-8H-dibenzo[a,i]xanthene-8,13(14H)-diones derived from lawsone. Research on Chemical Intermediates, 2021, 47, 2207.	2.7	9
42	Adsorption of synâ^'propanethial Sâ^'oxide on the Zn₁₂O₁₂ cluster: insights from ab-initio modelling. Journal of Sulfur Chemistry, 2021, 42, 308-321.	2.0	1
43	Conformational analysis of 2,5â€diarylâ€4â€methylâ€2, 4â€dihydroâ€3 H â€1,2,4â€triazolâ€3â€ones: Multinuclear NMR and DFT calculations. Journal of Heterocyclic Chemistry, 2021, 58, 1130-1140.	2.6	0
44	IR and NMR properties of N-base:PH2F:BeX2 ternary and corresponding binary complexes stabilised by pnicogen and beryllium bonds. Molecular Physics, 2021, 119, e1905191.	1.7	8
45	A 13C chemical shifts study of iodopyrazoles: experimental results and relativistic and non-relativistic calculations. Structural Chemistry, 2021, 32, 925-937.	2.0	1
46	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. ChemPhysChem, 2021, 22, 764-774.	2.1	2
47	Carboranes as Lewis Acids: Tetrel Bonding in CB11H11 Carbonium Ylide. Crystals, 2021, 11, 391.	2.2	6
48	Transitionâ€metalâ€catalyzed dehydrogenative coupling of alcohols and amines: A novel and atomâ€economical access to amides. Journal of the Chinese Chemical Society, 2021, 68, 723-737.	1.4	25
49	Perturbing the Oâ€“Hâ€¦O Hydrogen Bond in 1-oxo-3-hydroxy-2-propene. Molecules, 2021, 26, 3086.	3.8	1
50	The Electrophilicities of XCF 3 and XCl (X=H, Cl, Br, I) and the Propensity of These Molecules To Form Hydrogen and Halogen Bonds with Lewis Bases: An Ab Initio Study. ChemPlusChem, 2021, 86, 778-784.	2.8	6
51	Evaluation of Electron Density Shifts in Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4741-4749.	2.5	15
52	Large Stabilization Effects by Intramolecular Beryllium Bonds in Ortho-Benzene Derivatives. Molecules, 2021, 26, 3401.	3.8	1
53	Reactivity of Coinage Metal Hydrides for the Production of H 2 Molecules. ChemistryOpen, 2021, 10, 724-730.	1.9	1
54	Alkylammonium Cation Affinities of Nitrogenated Organobases: The Roles of Hydrogen Bonding and Proton Transfer. ChemPlusChem, 2021, 86, 1097-1105.	2.8	0

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55	The SN2 reaction and its relationship with the Walden inversion, the Finkelstein and Menshutkin reactions together with theoretical calculations for the Finkelstein reaction. Structural Chemistry, 2021, 32, 1755-1761.	2.0	5
56	Clustering of Electron Deficient Bâ€•and Beâ€Containing Analogues: In the Fight for Tetracoordination, Beryllium Takes the Lead. European Journal of Inorganic Chemistry, 2021, 2021, 4393-4401.	2.0	2
57	Sequestration of Carbon Dioxide with Frustrated Lewis Pairs Based on N-Heterocycles with Silane/Germane Groups. Journal of Physical Chemistry A, 2021, 125, 6976-6984.	2.5	14
58	Investigation of fused remote N-heterocyclic silylenes (frNHSis), at DFT. Journal of Molecular Modeling, 2021, 27, 299.	1.8	0
59	The mechanism of the reaction of hydrazines with Î±,Î²-unsaturated carbonyl compounds to afford hydrazones and 2-pyrazolines (4,5-dihydro-1H-pyrazoles): Experimental and theoretical results. Tetrahedron, 2021, 97, 132413.	1.9	5
60	Stationary states of systems with intermolecular interactions dominated by electrostatics: Structure of trimethylammonium and tetramethylammonium chlorides and bromides in the gas phase, monomers and dimers. Chemical Physics Letters, 2021, 778, 138809.	2.6	2
61	How Aromatic Fluorination Exchanges the Interaction Role of Pyridine with Carbonyl Compounds: The Formaldehyde Adduct. Chemistry - A European Journal, 2021, 27, 13870-13878.	3.3	6
62	Direct synthesis of sulfenamides, sulfinamides, and sulfonamides from thiols and amines. RSC Advances, 2021, 11, 32394-32407.	3.6	17
63	Alkoxysulfenylation of alkenes: development and recent advances. RSC Advances, 2021, 11, 32513-32525.	3.6	7
64	Hydroxysulfonylation of alkenes: an update. RSC Advances, 2021, 11, 21651-21665.	3.6	13
65	Tetranuclear copper(ii) cubane complexes derived from self-assembled 1,3-dimethyl-5-(o-phenolate-azo)-6-aminouracil: structures, non-covalent interactions and magnetic property. New Journal of Chemistry, 2021, 45, 2742-2753.	2.8	9
66	Recent advances in intermolecular 1,2-difunctionalization of alkenes involving trifluoromethylthiolation. RSC Advances, 2021, 11, 24474-24486.	3.6	18
67	Direct halosulfonylation of alkynes: an overview. RSC Advances, 2021, 11, 33447-33460.	3.6	24
68	Substitution effects via aromaticity, polarizability, APT, AIM, IR analysis, and hydrogen adsorption in C20-nTin nanostructures: a DFT survey. Journal of Molecular Modeling, 2021, 27, 348.	1.8	6
69	Recent trends in dehydroxylative trifluoro-methylation, -methoxylation, -methylthiolation, and -methylselenylation of alcohols. RSC Advances, 2021, 11, 39593-39606.	3.6	7
70	Anion Complexation Strongly Influences the Reactivity of Octafluorocyclooctatetraene. ChemistrySelect, 2021, 6, 13897-13905.	1.5	0
71	Methods for the direct synthesis of thioesters from aldehydes: a focus review. Journal of Sulfur Chemistry, 2020, 41, 96-115.	2.0	33
72	Theoretical calculations of the chemical shifts of cyclo[n]phosphazenes for n = 2, 3, 4 and 5 (X₂PN)_n with Xâ€‰=â€‰CH₃, F, Cl and Br: the effect of relativistic corrections. Phosphorus, Sulfur and Silicon and the Related Elements, 2020, 195, 307-313.	1.6	6

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73	Fluorescence mechanism switching from ICT to PET by substituent chemical manipulation: Macrophage cytoplasm imaging probes. Dyes and Pigments, 2020, 175, 108172.	3.7	11
74	Aryl sulfonyl chlorides and sodium aryl sulfinates: non-volatile, non-stench, and non-toxic aryl thiol surrogates for direct aryl-sulfenylation of Câ€“H bonds. Journal of Sulfur Chemistry, 2020, 41, 210-228.	2.0	20
75	A theoretical and spectroscopic (NMR and IR) study of indirubin in solution and in the solid state. Journal of Physical Organic Chemistry, 2020, 33, e4043.	1.9	5
76	A density functional theory outlook on the possible sensing ability of boron nitride nanotubes and their Al- and Si-doped derivatives for sulfonamide drugs. Journal of Sulfur Chemistry, 2020, 41, 82-95.	2.0	12
77	Theoretical studies of perimidine and its derivatives: structures, energies, and spectra. Structural Chemistry, 2020, 31, 25-35.	2.0	4
78	Cross-dehydrogenative Coupling Reactions Between Formamidic C(sp2)â€“H and Xâ€“H (Xâ€‰=â€‰C, O, N) Bonds. Topics in Current Chemistry, 2020, 378, 46.	5.8	15
79	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. ChemPhysChem, 2020, 21, 2557-2563.	2.1	11
80	A relative energy gradient (REG) study of the nitrogen inversion in N-substituted aziridines. Chemical Physics Letters, 2020, 758, 137927.	2.6	4
81	Direct sulfonamidation of (hetero)aromatic Câ€“H bonds with sulfonyl azides: a novel and efficient route toN-(hetero)aryl sulfonamides. RSC Advances, 2020, 10, 37299-37313.	3.6	36
82	A C(Ï€-hole)â‹¯Clâ€“Zn tetrel interaction driving a metalâ€“organic supramolecular assembly. CrystEngComm, 2020, 22, 6979-6982.	2.6	2
83	A Computational Study of Metallacycles Formed by Pyrazolate Ligands and the Coinage Metals M = Cu(I), Ag(I) and Au(I): (pzM)n for n = 2, 3, 4, 5 and 6. Comparison with Structures Reported in the Cambridge Crystallographic Data Center (CCDC). Molecules, 2020, 25, 5108.	3.8	8
84	Diborane Concatenation Leads to New Planar Boron Chemistry. ChemPhysChem, 2020, 21, 2460-2467.	2.1	17
85	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
86	An ab initio investigation of alkaliâ€“metal non-covalent bonds Bâ‹¯LiR and Bâ‹¯NaR (R = F, H or) Tj ETQq0 0 0 rgBT /Overlock 10 T CH₃. Physical Chemistry Chemical Physics, 2020, 22, 16421-16430.	2.8	9
87	Probing the structures, binding energies, and spin-spin coupling constants of halogen-bonded Azine:ClF complexes. Chemical Physics Letters, 2020, 761, 137916.	2.6	12
88	Regiospecific Synthesis and Structural Studies of 3,5-Dihydro-4H-pyrido[2,3-b][1,4]diazepin-4-ones and Comparison with 1,3-Dihydro-2H-benzo[b][1,4]diazepin-2-ones. ACS Omega, 2020, 5, 25408-25422.	3.5	5
89	The Importance of Strain (Preorganization) in Beryllium Bonds. Molecules, 2020, 25, 5876.	3.8	2
90	Interaction between Trinuclear Regium Complexes of Pyrazolate and Anions, a Computational Study. International Journal of Molecular Sciences, 2020, 21, 8036.	4.1	7

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91	Hybrid Boron-Carbon Chemistry. Molecules, 2020, 25, 5026.	3.8	5
92	Perimidines: a unique Ï€-amphoteric heteroaromatic system. Russian Chemical Reviews, 2020, 89, 1204-1260.	6.5	10
93	Cavity-trapped electrons: lithium doped tetracyano-2,6-naphthoquinodimethane (TNAP) systems. Journal of Molecular Modeling, 2020, 26, 118.	1.8	0
94	Hydrogen vs. Halogen Bonds in 1-Halo-Closo-Carboranes. Materials, 2020, 13, 2163.	2.9	10
95	N-Fluorobenzenesulfonimide: a useful and versatile reagent for the direct fluorination and amination of (hetero)aromatic Câ€“H bonds. RSC Advances, 2020, 10, 16756-16768.	3.6	43
96	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie, 2020, 132, 17635-17640.	2.0	21
97	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	13.8	136
98	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in Xâ€“Yâ€“X (X = B, Al;) Tj ETQq0 0 0 rgBT /Overlock	2.8	2
99	Environment-Sensitive Probes for Illuminating Amyloid Aggregation In Vitro and in Zebrafish. ACS Sensors, 2020, 5, 2792-2799.	7.8	21
100	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. Journal of Physical Chemistry A, 2020, 124, 5871-5878.	2.5	13
101	Anionâ€Anion Complexes Established between Aspartate Dimers. ChemPhysChem, 2020, 21, 1052-1059.	2.1	17
102	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	2.2	289
103	Supramolecular lead(<scp>ii</scp>) architectures engineered by tetrel bonds. CrystEngComm, 2020, 22, 2389-2396.	2.6	29
104	Direct Amination of Aromatic Câ€“H Bonds with Free Amines. Topics in Current Chemistry, 2020, 378, 37.	5.8	32
105	Complexes Between Adamantane Analogues B4X6 -X = {CH2, NH, O ; SiH2, PH, S} - and Dihydrogen, B4X6:nH2 (n = 1â€“4). Molecules, 2020, 25, 1042.	3.8	4
106	An Interacting Quantum Atoms (IQA) and Relative Energy Gradient (REG) Study of the Halogen Bond with Explicit Analysis of Electron Correlation. Molecules, 2020, 25, 2674.	3.8	14
107	A GIPAW versus GIAO-ZORA-SO study of 13C and 15N CPMAS NMR chemical shifts of aromatic and heterocyclic bromo derivatives. Solid State Nuclear Magnetic Resonance, 2020, 108, 101676.	2.3	5
108	Unusual Complexes of P(CH)3 with FH, ClH, and ClF. Molecules, 2020, 25, 2846.	3.8	1

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109	Hydrogen bonds and halogen bonds in complexes of carbones Lâ†'Câ†Ł as electron donors to HF and ClF, for L = CO, N2, HNC, PH3, and SH2. Physical Chemistry Chemical Physics, 2020, 22, 15966-15975.	2.8	5
110	From Very Strong to Inexistent Beâ^'Be Bonds in the Interactions of Be₂ with Ï€â€Systems. ChemPhysChem, 2020, 21, 2701-2708.	2.1	5
111	Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N2, OH2, NCH, SH2,) Tj ETQq1 1 0.784314 rgBT /	2.2	17
112	Oxidative carboxylation of olefins with CO₂: environmentally benign access to five-membered cyclic carbonates. RSC Advances, 2020, 10, 9103-9115.	3.6	27
113	Complexes H2CO:PXH2and HCO2Hâ€‰:â€‰PXH2for X=NC, F, Cl, CN, OH, CCH, CH3, and H: Pnicogen Bonds and Hydrogen Bonds. ChemPhysChem, 2020, 21, 741-748.	2.1	6
114	A Conceptual DFT Study of Phosphonate Dimers: Dianions Supported by H-Bonds. Journal of Physical Chemistry A, 2020, 124, 2207-2214.	2.5	25
115	Borophene as an electronic sensor for metronidazole drug: A computational study. Journal of Molecular Graphics and Modelling, 2020, 96, 107539.	2.4	64
116	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. Journal of Physical Chemistry A, 2020, 124, 1515-1521.	2.5	3
117	An experimental and computational NMR study of organometallic nineâ€membered rings: Trinuclear silver(I) complexes of pyrazolate ligands. Magnetic Resonance in Chemistry, 2020, 58, 319-328.	1.9	10
118	Calculated coupling constants ¹J(Xâ€“Y) and ¹K(Xâ€“Y), and fundamental relationships among the reduced coupling constants for molecules H_mXâ€“YH_n, with X, Y â••¹H, ⁷Li, ⁹Be, ¹¹B, ¹³C, ¹⁵N, ¹⁷O, ¹⁹F, ³¹P, ³³S, and ³⁵Cl. Magnetic Resonance in Chemistry, 2020, 58, 727-732.	1.9	0
119	Metastable Dianions and Dications. ChemPhysChem, 2020, 21, 1597-1607.	2.1	16
120	Stabilisation of dianion dimers trapped inside cyanostar macrocycles. Physical Chemistry Chemical Physics, 2020, 22, 11348-11353.	2.8	17
121	A DFT study on the sulfanilamide interaction with graphyne-like boron nitride nanosheet. Journal of Sulfur Chemistry, 2020, 41, 483-497.	2.0	16
122	Theoretical and Spectroscopic Characterization of API-Related Azoles in Solution and in Solid State. Current Pharmaceutical Design, 2020, 26, 4847-4857.	1.9	2
123	Recent Advances in the Application of Nanometal Catalysts for Glaser Coupling. Current Organic Chemistry, 2020, 23, 2489-2503.	1.6	20
124	Complexes between bicyclic boron derivatives and dihydrogen: the importance of strain. Structural Chemistry, 2020, 31, 1273-1279.	2.0	2
125	Withdrawal Notice: Recent Advances in Sonogashira Cross-Coupling Reactions Under Solvent-Free Conditions. Current Organic Chemistry, 2020, 24, .	1.6	0
126	Methods for direct C(sp2)â€“H bonds azidation. RSC Advances, 2019, 9, 25199-25215.	3.6	31

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127	Potential Energy Surfaces of HN(CH)SX:CO₂ for X = F, Cl, NC, CN, CCH, and H: NÂ·Â·Â·C Tetrel Bonds and OÂ·Â·Â·S Chalcogen Bonds. Journal of Physical Chemistry A, 2019, 123, 7270-7277.	2.5	23
128	Prototropic tautomerism of the addition products of N-heterocyclic carbenes to CO2, CS2, and COS. Structural Chemistry, 2019, 30, 1971-1979.	2.0	6
129	Systematic behaviour of electron redistribution on formation of halogen-bonded complexes Bâ‹¯XY, as determinedviaXY halogen nuclear quadrupole coupling constants. Physical Chemistry Chemical Physics, 2019, 21, 16914-16922.	2.8	3
130	Theoretical study of some Î»⁵â€phosphinines and their NMR spectra. Magnetic Resonance in Chemistry, 2019, 57, 975-981.	1.9	5
131	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. Journal of Physical Chemistry A, 2019, 123, 7124-7132.	2.5	24
132	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au 2 :HX Complexes. ChemPhysChem, 2019, 20, 1552-1552.	2.1	4
133	Cross-Dehydrogenative Coupling Reactions Between C(sp)â€“H and Xâ€“H (Xâ€‰=â€‰N, P, S, Si, Sn) Bonds: An Environmentally Benign Access to Heteroatom-Substituted Alkynes. Topics in Current Chemistry, 2019, 377, 20.	5.8	39
134	A structural study of new tetrakis(1H-pyrazol-1-yl)methanes. Tetrahedron, 2019, 75, 130690.	1.9	2
135	Sequestration of CO₂ by Phosphatrane Molecules. ChemPhysChem, 2019, 20, 3195-3200.	2.1	9
136	What Types of Noncovalent Bonds Stabilize Dimers (XCP)₂, for X = CN, Cl, F, and H?. Journal of Physical Chemistry A, 2019, 123, 10086-10094.	2.5	6
137	The synergy of different solid-state techniques to elucidate the supramolecular assembly of two 1H-benzotriazole polymorphs. Physical Chemistry Chemical Physics, 2019, 21, 19879-19889.	2.8	4
138	Nâ€¦C and Sâ€¦S Interactions in Complexes, Molecules, and Transition Structures HN(CH)SX:SCO, for X = F, Cl, NC, CCH, H, and CN. Molecules, 2019, 24, 3232.	3.8	4
139	Theoretical studies of conformational analysis and intramolecular dynamic phenomena. Structural Chemistry, 2019, 30, 2029-2055.	2.0	1
140	Recent advances in direct trifluoromethylation of olefinic Câ€“H bonds. RSC Advances, 2019, 9, 27625-27639.	3.6	38
141	The strange case of achiral compounds which were reported to always crystallize in the same chiral group. Structural Chemistry, 2019, 30, 633-636.	2.0	3
142	Cooperative Effects in Weak Interactions: Enhancement of Tetrel Bonds by Intramolecular Hydrogen Bonds. Molecules, 2019, 24, 308.	3.8	20
143	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	1.0	36
144	A DFT study on nanocones, nanotubes (4,0), nanosheets and fullerene C₆₀ as anodes in Mg-ion batteries. RSC Advances, 2019, 9, 853-862.	3.6	29

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145	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	2.8	13
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