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	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.	1.1	0
2	Stand up for Electrostatics: The Disiloxane Case. ChemPhysChem, 2022, 23, .	1.0	3
3	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.	1.8	3
4	A DFT study of the tautomerism of 1H-benzo[de]cinnolines and their protonated forms. Theoretical Chemistry Accounts, 2022, 141, 1.	0.5	2
5	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.	1.7	2
6	Theoretical study of the NO₃radical reaction with CH₂ClBr, CH₂ICl, CH₂BrI, CHCl₂Br, and CHClBr₂. Physical Chemistry Chemical Physics, 2022, 24, 14365-14374.	1.3	3
7	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.	1.7	3
8	Use of 5,10â€Disubstituted Dibenzoazaborines and Dibenzophosphaborines as Cyclic Supports of Frustrated Lewis Pairs for the Capture of CO₂. ChemPhysChem, 2022, 23, .	1.0	6
9	Multinuclear magnetic resonance studies of five silver(I) trinuclear pyrazolate complexes. Structural Chemistry, 2021, 32, 215-224.	1.0	3
10	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.	1.1	4
11	Spontaneous bond dissociation cascades induced by Be_n clusters (n = 2,4). Physical Chemistry Chemical Physics, 2021, 23, 6448-6454.	1.3	3
12	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	1.4	1
13	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.	1.4	0
14	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.	0.8	8
15	A 13C chemical shifts study of iodopyrazoles: experimental results and relativistic and non-relativistic calculations. Structural Chemistry, 2021, 32, 925-937.	1.0	1
16	A Density Functional Theory Study of Optical Rotation in Some Aziridine and Oxirane Derivatives. ChemPhysChem, 2021, 22, 764-774.	1.0	2
17	HÃ¼ckeloid model for planar boranes. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	4
18	Perturbing the Oâ€“Hâ€¦O Hydrogen Bond in 1-oxo-3-hydroxy-2-propene. Molecules, 2021, 26, 3086.	1.7	1

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19	Evaluation of Electron Density Shifts in Noncovalent Interactions. Journal of Physical Chemistry A, 2021, 125, 4741-4749.	1.1	15
20	Large Stabilization Effects by Intramolecular Beryllium Bonds in Ortho-Benzene Derivatives. Molecules, 2021, 26, 3401.	1.7	1
21	Reactivity of Coinage Metal Hydrides for the Production of H 2 Molecules. ChemistryOpen, 2021, 10, 724-730.	0.9	1
22	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.	1.0	5
23	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.	1.0	2
24	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.	1.1	14
25	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.	1.2	2
26	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.	0.8	6
27	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.	0.9	5
28	Rivalry between Regium and Hydrogen Bonds Established within Diatomic Coinage Molecules and Lewis Acids/Bases. ChemPhysChem, 2020, 21, 2557-2563.	1.0	11
29	A C(ï€-hole)â‹¯Clâ€“Zn tetrel interaction driving a metalâ€“organic supramolecular assembly. CrystEngComm, 2020, 22, 6979-6982.	1.3	2
30	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.	1.7	8
31	Diborane Concatenation Leads to New Planar Boron Chemistry. ChemPhysChem, 2020, 21, 2460-2467.	1.0	17
32	Probing the structures, binding energies, and spin-spin coupling constants of halogen-bonded Azine:ClF complexes. Chemical Physics Letters, 2020, 761, 137916.	1.2	12
33	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.	1.6	5
34	The Importance of Strain (Preorganization) in Beryllium Bonds. Molecules, 2020, 25, 5876.	1.7	2
35	Interaction between Trinuclear Regium Complexes of Pyrazolate and Anions, a Computational Study. International Journal of Molecular Sciences, 2020, 21, 8036.	1.8	7
36	Hybrid Boron-Carbon Chemistry. Molecules, 2020, 25, 5026.	1.7	5

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37	Perimidines: a unique Ï€-amphoteric heteroaromatic system. Russian Chemical Reviews, 2020, 89, 1204-1260.	2.5	10
38	Spodium Bonds: Noncovalent Interactions Involving Groupâ€…12 Elements. Angewandte Chemie - International Edition, 2020, 59, 17482-17487.	7.2	136
39	Bonding between electron-deficient atoms: strong Lewis-acid character preserved in Xâ€“Yâ€“X (X = B, Al;) Tj ETQq1 1 0.784314 rgBT	1.4	2
40	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. Journal of Physical Chemistry A, 2020, 124, 5871-5878.	1.1	13
41	Not Only Hydrogen Bonds: Other Noncovalent Interactions. Crystals, 2020, 10, 180.	1.0	289
42	Complexes Between Adamantane Analogues B4X6 -X = {CH2, NH, O ; SiH2, PH, S} - and Dihydrogen, B4X6:nH2 (n = 1â€“4). Molecules, 2020, 25, 1042.	1.7	4
43	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.	1.5	5
44	Hydrogen bonds and halogen bonds in complexes of carbones Lâ†’Câ†L as electron donors to HF and ClF, for L = CO, N2, HNC, PH3, and SH2. Physical Chemistry Chemical Physics, 2020, 22, 15966-15975.	1.3	5
45	From Very Strong to Inexistent Beâ”Be Bonds in the Interactions of Be₂ with Ï€â€Systems. ChemPhysChem, 2020, 21, 2701-2708.	1.0	5
46	Regium Bonds between Silver(I) Pyrazolates Dinuclear Complexes and Lewis Bases (N2, OH2, NCH, SH2,) Tj ETQq0 0 0 rgBT /Overlock 10	1.0	17
47	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.	1.0	6
48	A Conceptual DFT Study of Phosphonate Dimers: Dianions Supported by H-Bonds. Journal of Physical Chemistry A, 2020, 124, 2207-2214.	1.1	25
49	Are Anions of Cyclobutane Beryllium Derivatives Stabilized through Four-Center One-Electron Bonds?. Journal of Physical Chemistry A, 2020, 124, 1515-1521.	1.1	3
50	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.	1.1	10
51	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.	1.1	0
52	Metastable Dianions and Dications. ChemPhysChem, 2020, 21, 1597-1607.	1.0	16
53	Stabilisation of dianion dimers trapped inside cyanostar macrocycles. Physical Chemistry Chemical Physics, 2020, 22, 11348-11353.	1.3	17
54	Theoretical and Spectroscopic Characterization of API-Related Azoles in Solution and in Solid State. Current Pharmaceutical Design, 2020, 26, 4847-4857.	0.9	2

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55	Complexes between bicyclic boron derivatives and dihydrogen: the importance of strain. Structural Chemistry, 2020, 31, 1273-1279.	1.0	2
56	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.	1.1	23
57	Prototropic tautomerism of the addition products of N-heterocyclic carbenes to CO2, CS2, and COS. Structural Chemistry, 2019, 30, 1971-1979.	1.0	6
58	Theoretical study of some Î»⁵â€phosphinines and their NMR spectra. Magnetic Resonance in Chemistry, 2019, 57, 975-981.	1.1	5
59	Weak Interactions Get Strong: Synergy between Tetrel and Alkaline-Earth Bonds. Journal of Physical Chemistry A, 2019, 123, 7124-7132.	1.1	24
60	A structural study of new tetrakis(1H-pyrazol-1-yl)methanes. Tetrahedron, 2019, 75, 130690.	1.0	2
61	Sequestration of CO₂ by Phosphatrane Molecules. ChemPhysChem, 2019, 20, 3195-3200.	1.0	9
62	Synthesis of ¹⁵Nâ€labelled 3,5â€dimethylpyridine. Journal of Labelled Compounds and Radiopharmaceuticals, 2019, 62, 914-919.	0.5	1
63	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.	1.1	6
64	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.	1.3	4
65	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.	1.7	4
66	Theoretical studies of conformational analysis and intramolecular dynamic phenomena. Structural Chemistry, 2019, 30, 2029-2055.	1.0	1
67	The strange case of achiral compounds which were reported to always crystallize in the same chiral group. Structural Chemistry, 2019, 30, 633-636.	1.0	3
68	Cooperative Effects in Weak Interactions: Enhancement of Tetrel Bonds by Intramolecular Hydrogen Bonds. Molecules, 2019, 24, 308.	1.7	20
69	The beryllium bond. Advances in Inorganic Chemistry, 2019, 73, 73-121.	0.4	36
70	Modulating the intrinsic reactivity of molecules through non-covalent interactions. Physical Chemistry Chemical Physics, 2019, 21, 2222-2233.	1.3	13
71	Assignment of ¹H and ¹³C NMR data for three pairs of diastereomers of 4â€²â€X benzo[1,3]cyclopropa[1,2â€b]chromeneâ€4,5â€diones (XÂ=ÂH, OCH₃, and Cl). Magnetic Resonance in Chemistry, 2019, 57, 512-521.	1.1	3
72	Exploring N C tetrel and O S chalcogen bonds in HN(CH)SX:OCS systems, forâ€¯Xâ€¯=â€¯F, NC, Cl, CN, CCH, and H. Chemical Physics Letters, 2019, 730, 466-471.	1.2	22

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73	Ternary Complexes Stabilized by Chalcogen and Alkalineâ€Earth Bonds: Crucial Role of Cooperativity and Secondary Noncovalent Interactions. Chemistry - A European Journal, 2019, 25, 11688-11695.	1.7	20
74	Can a Clâ€“HÂ·Â·Â·F Hydrogen Bond Replace a ClÂ·Â·Â·F Halogen Bond? H2XP:ClY:ZH versus H2XP:ClY:HZ for Y, Z = F, Cl. Journal of Physical Chemistry A, 2019, 123, 3992-3999.	1.1	1
75	The extraordinary richness of the reaction between diazomethane and tetracyanoethylene: can computational calculations shed light on old papers?. New Journal of Chemistry, 2019, 43, 7831-7838.	1.4	1
76	Gas-phase reactivity tuned through the interaction with alkaline-earth derivatives. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	5
77	The structure of the anti-aging agent J147 used for treating Alzheimer's disease. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 271-276.	0.2	3
78	Multinuclear NMR spectra and GIAO/DFT calculations of N-benzylazoles and N-benzylbenzazoles. Structural Chemistry, 2019, 30, 1729-1735.	1.0	10
79	Understanding Regium Bonds and their Competition with Hydrogen Bonds in Au₂:HX Complexes. ChemPhysChem, 2019, 20, 1572-1580.	1.0	38
80	Probing Câ‹¯S chalcogen bonds in complexes SC:SHX, for Xâ€¯=â€¯NO2, NC, F, Cl, CN, CCH, and NH2. Chemical Physics Letters, 2019, 721, 86-90.	1.2	8
81	An Example of Polynomial Expansion: The Reaction of 3(5)-Methyl-1H-Pyrazole with Chloroform and Characterization of the Four Isomers. Molecules, 2019, 24, 568.	1.7	6
82	Cations brought together by hydrogen bonds: the protonated pyridineâ€“boronic acid dimer explained. Physical Chemistry Chemical Physics, 2019, 21, 5796-5802.	1.3	33
83	Modulating intramolecular chalcogen bonds in aromatic (thio)(seleno)phene-based derivatives. Physical Chemistry Chemical Physics, 2019, 21, 23645-23650.	1.3	20
84	Relativistic Effects on NMR Parameters of Halogen-Bonded Complexes. Molecules, 2019, 24, 4399.	1.7	11
85	Pnicogen bonds in complexes with CO and CS: differentiating properties. Molecular Physics, 2019, 117, 1117-1127.	0.8	14
86	Interaction of Nâ€Heterocyclic Carbenes and Simple Carbenes with Small Molecules (One to) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2019, 56, 359-370.	1.4	9
87	A theoretical NMR study of polymorphism in crystal structures of azoles and benzazoles. Magnetic Resonance in Chemistry, 2019, 57, 275-284.	1.1	9
88	Synthesis, structure and NMR study of fluorinated isoxazoles derived from hemi-curcuminoids. Journal of Fluorine Chemistry, 2019, 219, 39-49.	0.9	5
89	Reaction of ClF and Cl2 with PH2X: The oxidation of P(III) to P(V). Chemical Physics Letters, 2019, 715, 190-194.	1.2	4
90	About the statistical analysis of theoretically calculated values. Structural Chemistry, 2019, 30, 283-287.	1.0	1

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91	Complexes between H₂ and neutral oxyacid beryllium derivatives. The role of angular strain. Molecular Physics, 2019, 117, 1142-1150.	0.8	5
92	New N,C-Diaryl-1,2,4-triazol-3-ones: Synthesis and Evaluation as Anticancer Agents. Medicinal Chemistry, 2019, 15, 360-372.	0.7	5
93	Hydrogen and Halogen Bonding in Cyclic FH_(4-n):FCl_n Complexes, for n = 0â€“4. Journal of Physical Chemistry A, 2018, 122, 2587-2597.	1.1	16
94	Weak interactions and cooperativity effects on disiloxane: a look at the building block of silicones. Molecular Physics, 2018, 116, 1539-1550.	0.8	10
95	Beâ€•and Mgâ€Based Electron and Anion Sponges. ChemPhysChem, 2018, 19, 1701-1706.	1.0	8
96	The structures of 1,4-diaryl-5-trifluoromethyl-1H-1,2,3-triazoles related to J147, a drug for treating Alzheimer's disease. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 513-522.	0.2	8
97	Complexes of O=C=S with Nitrogen Bases: Chalcogen Bonds, Tetrel Bonds, and Other Secondary Interactions. ChemPhysChem, 2018, 19, 1886-1894.	1.0	24
98	Synthesis, Structure and Anion Sensing Properties of a Dicationic Bis(imidazolium)â€Based Cyclophane. ChemistrySelect, 2018, 3, 3855-3859.	0.7	7
99	A vibrational circular dichroism (VCD) methodology for the measurement of enantiomeric excess in chiral compounds in the solid phase and for the complementary use of NMR and VCD techniques in solution: the camphor case. Analyst, The, 2018, 143, 1406-1416.	1.7	19
100	Trapping One Electron between Three Beryllium Atoms: Very Strong Oneâ€Electron Threeâ€Center Bonds. ChemPhysChem, 2018, 19, 1068-1074.	1.0	6
101	Hydrogen-Bonding Acceptor Character of Be₃, the Beryllium Three-Membered Ring. Journal of Physical Chemistry A, 2018, 122, 1472-1478.	1.1	15
102	Alkaline-earth (Be, Mg and Ca) bonds at the origin of huge acidity enhancements. Physical Chemistry Chemical Physics, 2018, 20, 2413-2420.	1.3	32
103	Are beryllium-containing biphenyl derivatives efficient anion sponges?. Journal of Molecular Modeling, 2018, 24, 16.	0.8	7
104	Fostering the Basic Instinct of Boron in Boronâ€“Beryllium Interactions. Journal of Physical Chemistry A, 2018, 122, 3313-3319.	1.1	8
105	The structure of 2,4,6-tris(1Hâ€“pyrazol-1-yl)-1,3,5-triazine in the solid state: on polymorphs, pseudopolymorphs and co-crystals. Structural Chemistry, 2018, 29, 15-21.	1.0	3
106	Molecular structure in the solid state by X-ray crystallography and SSNMR and in solution by NMR of two 1,4-diazepines. Journal of Molecular Structure, 2018, 1155, 205-214.	1.8	7
107	A LFER analysis of the singlet-triplet gap in a series of sixty-six carbenes. Chemical Physics Letters, 2018, 691, 33-36.	1.2	20
108	The Structure of Nâ€phenylâ€pyrazoles and Indazoles: Mononitro, Dinitro, and Trinitro Derivatives. Journal of Heterocyclic Chemistry, 2018, 55, 44-64.	1.4	9

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109	A theoretical NMR study of selected benzazoles: Comparison of GIPAW and GIAOâ€PCM (DMSO) calculations. Magnetic Resonance in Chemistry, 2018, 56, 164-171.	1.1	14
110	Large Protonâ€Affinity Enhancements Triggered by Noncovalent Interactions. Chemistry - A European Journal, 2018, 24, 1971-1977.	1.7	15
111	Solvent and Substituent Effects on the Phosphine + CO2 Reaction. Inorganics, 2018, 6, 110.	1.2	17
112	A theoretical study of the properties of ninetyâ€two â€œaromaticâ€•sixâ€membered rings including benzene, azines, phosphinines and azaphosphinines. Heteroatom Chemistry, 2018, 29, .	0.4	14
113	The structure of four thallium tris(1H-pyrazol-1-yl)hydroborates in the solid state by X-ray crystallography and in solution by NMR and DFT-GIAO calculations. Inorganica Chimica Acta, 2018, 483, 402-410.	1.2	6
114	Using protonation to change a Clâ¯N halogen bond in N-Base:ClOH complexes to a Clâ¯O halogen bond. Chemical Physics Letters, 2018, 710, 123-128.	1.2	10
115	Complexes between neutral oxyacid beryllium salts and dihydrogen: a possible way for hydrogen storage?. Dalton Transactions, 2018, 47, 12516-12520.	1.6	7
116	From diiodo TrÃ¶ger's bases towards halogen-bonded porous organic crystalline materials. CrystEngComm, 2018, 20, 3167-3170.	1.3	9
117	Libration of phenyl groups detected by <scp>VTâ€SSNMR</scp>: Comparison with Xâ€ray crystallography. Magnetic Resonance in Chemistry, 2018, 56, 1083-1088.	1.1	2
118	Enhancement of Thermodynamic Gasâ€Phase Acidity and Basicity of Water by Means of Secondary Interactions. ChemPhysChem, 2018, 19, 2486-2491.	1.0	2
119	Intramolecular magnesium bonds in malonaldehyde-like systems: a critical view of the resonance-assisted phenomena. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	8
120	Complexes of CO2 with the Azoles: Tetrel Bonds, Hydrogen Bonds and Other Secondary Interactions. Molecules, 2018, 23, 906.	1.7	35
121	Binding indirect greenhouse gases OCS and CS2by nitrogen heterocyclic carbenes (NHCs). Physical Chemistry Chemical Physics, 2018, 20, 19552-19559.	1.3	20
122	A theoretical study of perovskites related to CH₃NH₃PbX₃ (X = F,) Tj ETQq0 0 0 rgBT /Overlock 1	1.4	12
123	Conformational aspects of polymorphs and phases of 2-propyl-1H-benzimidazole. IUCrJ, 2018, 5, 706-715.	1.0	7
124	The Hydrogen-bond Basicity of Carbenes. Croatica Chemica Acta, 2018, 91, .	0.1	2
125	Lone-Pair Hole on P: PÂ·Â·Â·N Pnicogen Bonds Assisted by Halogen Bonds. Journal of Physical Chemistry A, 2017, 121, 1362-1370.	1.1	31
126	Borylene as an electron-pair donor for Pâ€¦B pnicogen bonds. Structural Chemistry, 2017, 28, 1419-1427.	1.0	16

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127	A theoretical study of the H n F4â^'n Si:N-base (nÂ=Â1â€“4) tetrel-bonded complexes. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	27
128	The structure of N -arylindazoles and their aza-derivatives in the solid state: A systematic analysis of the Cambridge Structural Database coupled with DFT calculations. Journal of Molecular Structure, 2017, 1137, 186-192.	1.8	5
129	Hydrogen-bonded complexes with carbenes as electron-pair donors. Chemical Physics Letters, 2017, 675, 46-50.	1.2	20
130	Trapping CO₂ by Adduct Formation with Nitrogen Heterocyclic Carbenes (NHCs): A Theoretical Study. Chemistry - A European Journal, 2017, 23, 10604-10609.	1.7	45
131	Carbenes as Electron-Pair Donors To CO₂ for CÂ·Â·Â·C Tetrel Bonds and Câ€“C Covalent Bonds. Journal of Physical Chemistry A, 2017, 121, 4039-4047.	1.1	48
132	Curcumin Related 1,4â€Diazepines: Regioselective Synthesis, Structure Analysis, Tautomerism, NMR Spectroscopy, Xâ€ray Crystallography, Density Functional Theory and GIAO Calculations. ChemistrySelect, 2017, 2, 3732-3738.	0.7	6
133	Supramolecular organization of perfluorinated 1H-indazoles in the solid state using X-ray crystallography, SSNMR and sensitive (VCD) and non sensitive (MIR, FIR and Raman) to chirality vibrational spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 1632-1643.	1.3	18
134	Carbenes as Electronâ€Pair Donors for Pâ‹…â‹…â‹…C Pnicogen Bonds. ChemPhysChem, 2017, 18, 1597-1610.	1.0	24
135	The organic chemistry of poly(1H-pyrazol-1-yl)methanes. Coordination Chemistry Reviews, 2017, 339, 153-182.	9.5	34
136	Azines as Electron-Pair Donors to CO₂ for NÂ·Â·Â·C Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 8017-8025.	1.1	35
137	Carbonâ€“Carbon Bonding between Nitrogen Heterocyclic Carbenes and CO₂. Journal of Physical Chemistry A, 2017, 121, 8136-8146.	1.1	45
138	Modulating the Proton Affinity of Silanol and Siloxane Derivatives by Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 7424-7431.	1.1	16
139	Hydrogen Bond versus Halogen Bond in Cationâ€“Cation Complexes: Effect of the Solvent. ChemPhysChem, 2017, 18, 3462-3468.	1.0	34
140	The Curious Case of 2-Propyl-1H-benzimidazole in the Solid State: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 5665-5674.	1.1	14
141	Using one halogen bond to change the nature of a second bond in ternary complexes with Pâ‹¯Cl and Fâ‹¯Cl halogen bonds. Faraday Discussions, 2017, 203, 29-45.	1.6	17
142	Halogen bonding with carbene bases. Chemical Physics Letters, 2017, 685, 338-343.	1.2	16
143	Activation of Dinitrogen as A Dipolarophile in 1,3-Dipolar Cycloadditions: A Theoretical Study Using Nitrile Imines as â€œOctetâ€•1,3-Dipoles. Scientific Reports, 2017, 7, 6115.	1.6	10
144	Modulation of in:out and out:out conformations in [X.Xâ€².Xâ€²â€²] phosphatranes by Lewis acids. Physical Chemistry Chemical Physics, 2017, 19, 20647-20656.	1.3	3

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145	Beryllium-based fluorenes as efficient anion sponges. Physical Chemistry Chemical Physics, 2017, 19, 23052-23059.	1.3	10
146	Enhancing Intramolecular Chalcogen Interactions in 1-Hydroxy-8-YH-naphthalene Derivatives. Journal of Physical Chemistry A, 2017, 121, 8995-9003.	1.1	11
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