

Qingzhong Li

List of Publications by Year in descending order

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131
papers

2,636
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201674

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Chemical Origin of Termination-Functionalized MXenes: Ti_3C_2 as a Case Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19254-19261.	3.1	194
2	Cooperativity between the Halogen Bond and the Hydrogen Bond in $\text{H}_3\text{N}\cdots\text{XY}\cdots\text{HF}$ Complexes (X, Y=F, Cl, Br). <i>ChemPhysChem</i> , 2008, 9, 2265-2269.	2.1	152
3	A π -hole interaction with radical species as electron donors: does single-electron tetrel bonding exist?. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11617-11625.	2.8	113
4	Comparison of tetrel bonds in neutral and protonated complexes of pyridine and furan ($\text{T} = \text{C}, \text{Si}, \text{and Ge}$) with NH_3 . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 5550-5559.	2.8	98
5	A bioinspired hybrid membrane with wettability and topology anisotropy for highly efficient fog collection. <i>Journal of Materials Chemistry A</i> , 2019, 7, 124-132.	10.3	93
6	Competition between hydrogen bond and halogen bond in complexes of formaldehyde with hypohalous acids. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 6837.	2.8	92
7	Thermoresponsive Graphene Membranes with Reversible Gating Regularity for Smart Fluid Control. <i>Advanced Functional Materials</i> , 2019, 29, 1808501.	14.9	70
8	Comparative Strengths of Tetrel, Pnictogen, Chalcogen, and Halogen Bonds and Contributing Factors. <i>Molecules</i> , 2018, 23, 1681.	3.8	69
9	Tetrel bond of pseudohalide anions with XH_3F (X = C, Si, Ge, and Sn) and its role in $\text{S}_\text{N}2$ reaction. <i>Journal of Chemical Physics</i> , 2016, 145, 224310.	3.0	68
10	Prediction and characterization of the $\text{HMgH}\cdots\text{LiX}$ (X = H, OH, F, CCH, CN, and NC) complexes: a lithium hydride lithium bond. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2402.	2.8	64
11	Interplay between halogen bond and lithium bond in $\text{MCN}\cdots\text{LiCN}\cdots\text{XCCH}$ (M = H, Li, and Na; X = Cl, Br, and I) complex: The enhancement of halogen bond by a lithium bond. <i>Journal of Computational Chemistry</i> , 2011, 32, 3296-3303.	3.3	61
12	Carbene tetrel-bonded complexes. <i>Structural Chemistry</i> , 2017, 28, 823-831.	2.0	47
13	The π -Tetrel Bond and its Influence on Hydrogen Bonding and Proton Transfer. <i>ChemPhysChem</i> , 2018, 19, 736-743.	2.1	46
14	$\text{Se}\cdots\text{N}$ Chalcogen Bond and $\text{Se}\cdots\text{X}$ Halogen Bond Involving $\text{F}_2\text{C}\cdots\text{Se}$: Influence of Hybridization, Substitution, and Cooperativity. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3518-3527.	2.5	45
15	Ab Initio Study of Lithium-Bonded Complexes with Carbene as an Electron Donor. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14156-14160.	2.5	43
16	Theoretical Study of the Interplay between Lithium Bond and Hydrogen Bond in Complexes Involved with HLi and HCN . <i>ChemPhysChem</i> , 2009, 10, 3310-3315.	2.1	38
17	Cooperative and Diminutive Effects of Pnictogen Bonds and Cation- π Interactions. <i>ChemPhysChem</i> , 2014, 15, 500-506.	2.1	38
18	Comparison of π -Hole and σ -Hole Tetrel Bonds Formed by Pyrazine and 1,4-Dicyanobenzene: The Interplay between Anion- π and Tetrel Bonds. <i>ChemPhysChem</i> , 2017, 18, 2442-2450.	2.1	38

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37	Ultrahigh hydrogen storage capacity of novel porous aromatic frameworks. <i>Journal of Materials Chemistry A</i> , 2015, 3, 10724-10729.	10.3	23
38	Abnormal synergistic effects between Lewis acid–base interaction and halogen bond in $F_3C-NX_3-NCX_3$. <i>Molecular Physics</i> , 2015, 113, 3809-3814.	1.7	23
39	Comparison for σ -hole and π -hole tetrel-bonded complexes involving cyanoacetaldehyde. <i>Molecular Physics</i> , 2018, 116, 222-230.	1.7	22
40	Theoretical study of halogen–hydride halogen bonds in $F_3C-CL-Â-Â-Â-HM$ (L=Cl, Br; M=Li, BeH, $_2$). <i>Tj ETQq 0 0 rgBT /Overloc</i>	1.7	21
41	Competition between dihydrogen bond and beryllium bond in complexes between $HBeH$ and $HArF$: A huge blue shift of distant HAr stretch. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 90, 135-140.	3.9	21
42	Regulation of coin metal substituents and cooperativity on the strength and nature of tetrel bonds. <i>RSC Advances</i> , 2017, 7, 46321-46328.	3.6	20
43	Comparison of tetrel bonds and halogen bonds in complexes of DMSO with ZF_3X (Z = C). <i>Tj ETQq 1 0,784314 rgBT /Overloc</i>	3.6	19
44	Comparison of σ -hole and π -hole tetrel bonds in complexes of borazine with TH_3F and F_2TO/H_2TO (T = C, Si, Ge). <i>International Journal of Quantum Chemistry</i> , 2019, 2, 0119, e25910.	2.0	19
45	How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds. <i>RSC Advances</i> , 2015, 5, 12488-12497.	3.6	18
46	Synergistic and Diminutive Effects between Regium and Aerogen Bonds. <i>ChemPhysChem</i> , 2020, 21, 2426-2431.	2.1	17
47	Large blue shift of the $H-Ar$ stretching frequency in hydrogen- and halogen-bonded complexes of $HArF$ with dihalogen molecules. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 506-511.	3.9	16
48	Influence of the protonation of pyridine nitrogen on pnictogen bonding: competition and cooperativity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11348-11356.	2.8	16
49	Comparison between Hydrogen and Halogen Bonds in Complexes of $6OX$ -Fulvene with Pnictogen and Chalcogen Electron Donors. <i>ChemPhysChem</i> , 2019, 20, 1978-1984.	2.1	16
50	Theoretical study on the interlay of hydrogen bonds in the trimers involving HCN and water. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1396-1402.	2.0	15
51	Competition between σ -hole pnictogen bond and π -hole tetrel bond in complexes of $CF_2=CFZH_2$ (Z = P, As, and Sb). <i>Molecular Physics</i> , 2019, 117, 251-259.	1.7	15
52	The π -hole tetrel bond between X_2TO and CO_2 : Substituent effects and its potential adsorptivity for CO_2 . <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26251.	2.0	15
53	Weak σ -Hole Trel Bond between C_5H_5Tr (Tr=B, Al, Ga) and Haloethyne: Substituent and Cooperativity Effects. <i>ChemPhysChem</i> , 2021, 22, 481-487.	2.1	15
54	Influence of substituents on the nature of metal– π interaction and its cooperativity with halogen bond. <i>Journal of Chemical Physics</i> , 2015, 143, 054308.	3.0	14

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55	Triel-hydride triel bond between ZX_3 (Z = B and Al; X = H and Me) and $THMe_3$ (T) <i>J. Theoretical Chemistry</i> , 2019, 11, 1078-1149.	3.5	14
56	Coinage-Metal Bond between [1.1.1]Propellane and $M_2/MCl/MCH_3$ (M = Cu, Ag, and Au): Cooperativity and Substituents. <i>Molecules</i> , 2019, 24, 2601.	3.8	14
57	Hydrogen bond and π -hole interaction in $M_2C=S\hat{A}\hat{A}HCN$ (M = H, F, Cl, Br, HO, H_3C), <i>J. Theoretical Chemistry</i> , 2012, 112, 1491-1498.	2.0	13
58	Some measures for making a traditional halogen bond be chlorine-shared or ion-pair one in $FCl\hat{A}\hat{A}NH_3$ complex. <i>Molecular Physics</i> , 2016, 114, 3643-3649.	1.7	13
59	Non-additivity between substitution and cooperative effects in enhancing hydrogen bonds. <i>Journal of Chemical Physics</i> , 2014, 141, 244305.	3.0	11
60	Violation of Electrostatic Rules: Shifting the Balance between Pnictogen Bonds and Lone Pair- π Interactions Tuned by Substituents. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7288-7295.	2.5	11
61	Coinage metal dimers as the noncovalent interaction acceptors: study of the π -lump interactions. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21152-21161.	2.8	11
62	Comparison of triel bonds with different chalcogen electron donors: Its dependence on triel donor and methyl substitution. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26046.	2.0	11
63	Xe-chalcogen aerogen bond. Effect of substituents and size of chalcogen atom. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4115-4121.	2.8	11
64	Physicochemical Properties, 1H -NMR, Ab Initio Calculations and Molecular Interaction in Binary Mixtures of N-methylimidazole with Methanol. <i>Journal of Solution Chemistry</i> , 2018, 47, 1875-1901.	1.2	10
65	Competitive interaction between halogen and hydrogen bonds in $NH_2Br\hat{A}\hat{A}HOX$ (X = F, Cl, and I) <i>J. Theoretical Chemistry</i> , 2019, 11, 1078-1149.	2.0	9
66	Some measures for mediating the strengths of halogen bonds with the B-B bond in diborane(4) as an unconventional halogen acceptor. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 128-137.	2.0	9
67	Competition between halogen bond and hydrogen bond in complexes of superalkali Li_3S and halogenated acetylene $XCCH$ (X = F, Cl, Br, and I). <i>International Journal of Quantum Chemistry</i> , 2015, 115, 99-105.	2.0	9
68	Dinuclear first-row transition metal-hydrogen complexes: metal-metal and metal-ligand bonds determined by the d electron configuration of the metal atom. <i>New Journal of Chemistry</i> , 2016, 40, 1988-1996.	2.8	9
69	Abnormal Tetrel Bonds between Formamidine and TH_3F : Substituent Effects. <i>ChemistrySelect</i> , 2018, 3, 2842-2849.	1.5	9
70	Comparison of halide donors based on $\pi\hat{A}\hat{A}M$ (M = Cu, Ag, Au), $\pi\hat{A}\hat{A}H$ and $\pi\hat{A}\hat{A}$ -halogen bonds. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	1.4	9
71	A theoretical analysis of the weakly bound complexes $HM\hat{A}\hat{A}HXY$ (M=O and S; XY=CN and NC): comparison with $H_2M\hat{A}\hat{A}HXY$ complexes. <i>Molecular Physics</i> , 2010, 108, 1655-1664.	1.7	8
72	Ab initio study of the structure, cooperativity, and vibrational properties in the mixed hydrogen-bonded trimers of hydrogen isocyanide and water. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1072-1080.	2.0	8

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73	Ab initio study of synergetic effects of two strong interactions of cation-π interaction and lithium bond in M+@Ar...phenyl lithium@Ar...N (M = Li, Na, K; N = H ₂ O and NH ₃) complex. <i>Molecular Physics</i> , 2013, 111, 457-465.		
74	Influence of cooperativity on the frequency shift of the Ar-H stretch vibration in HARF complexes. <i>Molecular Physics</i> , 2013, 111, 497-504.	1.7	8
75	Synergic mechanism of an organic corrosion inhibitor for preventing carbon steel corrosion in chloride solution. <i>Journal Wuhan University of Technology, Materials Science Edition</i> , 2015, 30, 325-330.	1.0	8
76	Intramolecular Si...O Tetrel Bonding: Tuning of Substituents and Cooperativity. <i>ChemistrySelect</i> , 2017, 2, 11104-11112.	1.5	8
77	Dual function of the boron center of BH(CO) ₂ /BH(N ₂) ₂ in halogen- and triel-bonded complexes with hypervalent halogens. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 84, 118-124.	2.4	8
78	Reliable Comparison of Pnicogen, Chalcogen, and Halogen Bonds in Complexes of 6-OXF ₂ -Fulvene (X = F, Cl, Br, I). <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 1078-1087.	3.6	8
79	A quantum chemical study of the structures, stability, and spectroscopy of halogen- and hydrogen-bonded complexes between cyanoacetaldehyde and hypochlorous acids. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 121, 157-163.	3.9	7
80	Influence of F and Se substitution on the structures, stabilities and nature of the complexes between F ₂ CSe and HOX (X = F, Cl, Br, and I). <i>RSC Advances</i> , 2015, 5, 52667-52675.	3.6	7
81	Group 12 Carbonates and their Binary Complexes with Nitrogen Bases and FH ₂ Z Molecules (Z = P, As). <i>Journal of Molecular Graphics and Modelling</i> , 2019, 90, 1078-1087.	2.1	7
82	Theoretical study of the interaction between LiNH ₂ and HMgH. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 675-681.	2.0	6
83	Is a MH (M = Be and Mg) radical a better electron donor in halogen-hydride interaction?: A theoretical comparison with HMH. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1293-1298.	2.0	6
84	Complicated synergistic effects between metal-π interaction and halogen bonding involving MCCX. <i>RSC Advances</i> , 2015, 5, 105160-105168.	3.6	6
85	Theoretical Design of Near-Infrared Fluorescent Sensor for F Anion Detection Based on 10-Hydroxybenzo[<i>h</i>]quinoline Backbone. <i>ACS Omega</i> , 2019, 4, 10516-10523.	3.5	6
86	Effect of carbon hybridization in C-F bond as an electron donor in triel bonds. <i>Journal of Chemical Physics</i> , 2020, 153, 074304.	3.0	6
87	Complexes of HARF and AuX (X = F, Cl, Br, I). Comparison of H-bonds, halogen bonds, F-shared bonds and covalent bonds. <i>Applied Organometallic Chemistry</i> , 2020, 34, e5891.	3.5	6
88	Unusual substituent effects in the Tr-Te triel bond. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26526.	2.0	6
89	Cooperative effects between triel and halogen bonds in complexes of pyridine derivatives: An opposite effect of the nitrogen oxidation on triel and halogen bonds. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26429.	2.0	6
90	Enhancement of the Tetrel Bond by the Effects of Substituents, Cooperativity, and Electric Field: Transition from Noncovalent to Covalent Bond. <i>ChemPhysChem</i> , 2021, 22, 2305-2312.	2.1	6

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91	Chalcogen Bond Involving Zinc(II)/Cadmium(II) Carbonate and Its Enhancement by Spodium Bond. <i>Molecules</i> , 2021, 26, 6443.	3.8	6
92	Resonance-assisted intramolecular triel bonds. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 15015-15024.	2.8	6
93	Enhancing the function, non-additivity, and substitution position effect of the Li atom in the cation-π interaction and its mechanism: an ab initio study of Li-π-π-Li-substituted benzene complexes. <i>Molecular Physics</i> , 2012, 110, 65-74.	1.7	5
94	Theoretical study of synergistic effects between anion-π and metal-Lp interactions. <i>RSC Advances</i> , 2015, 5, 76912-76918.	3.6	5
95	Prediction and characterization of halogen bonds involving formamidine and its derivatives. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 195-202.	3.9	5
96	Structures of the phosphinidene germolenoid HP=GeLiF and its cycloaddition reaction with ethylene. <i>Structural Chemistry</i> , 2018, 29, 1647-1653.	2.0	5
97	Theoretical investigation of the nature of π(Bi, B)-M interactions in coinage metal π-diborene complexes. <i>New Journal of Chemistry</i> , 2021, 45, 13380-13388.	2.8	5
98	Comparative study on the nonadditivity of methyl group in lithium bonding and hydrogen bonding. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1127-1134.	2.0	4
99	Novel C-X halogen bonds in complexes of acetylene and its derivatives of Na and MPH3 (M=Cu, Ag, Au) with XCCF (X=Cl, Br, I). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 10-15.	3.9	4
100	Theoretical investigation of the addition reaction of the aluminum chlorosilylenoid H ₂ SiAlCl ₃ with ethylene. <i>Journal of Molecular Modeling</i> , 2016, 22, 150.	1.8	4
101	Diboron Bonds Between BX ₃ (X=H, F, CH ₃) and BYZ ₂ (Y=H, F; Z=CO, N ₂ , CNH). <i>ChemPhysChem</i> , 2021, 22, 1461-1469.	2.1	4
102	Tetrel Bonds between Phenyltrifluorosilane and Dimethyl Sulfoxide: Influence of Basis Sets, Substitution and Competition. <i>Molecules</i> , 2021, 26, 7231.	3.8	4
103	Halogen Bond Catalysis on Carbonyl-Olefin Ring-Closing Metathesis Reaction: Comparison with Lewis Acid Catalysis. <i>Chinese Journal of Chemistry</i> , 2022, 40, 1275-1284.	4.9	4
104	Insight into Spodium Bonding Characteristics of the MX ₂ -π (M = Zn, Cd and Hg; X = Cl, Br and I) Complexes: A Theoretical Study. <i>Molecules</i> , 2022, 27, 2885.	3.8	4
105	Novel non-covalent interactions involved with the Al ₁₃ M cluster (M = Li, Na, K, Cu, Ag.) <i>Tj ETQq1 1 0.784314 rgBT /Over</i>	1.7	3
106	Hydrogen bonding involved with superhalogen MX ₂ NY: its influence on the structure and stability of the superhalogen. <i>Molecular Physics</i> , 2014, 112, 1947-1953.	1.7	3
107	Enhancing effect of metal coordination interaction on pnictogen bonding. <i>Journal of Molecular Modeling</i> , 2016, 22, 64.	1.8	3
108	The ground and excited-state electronic structures of sandwich compounds Cp ₂ (ME) ₂ contain an (ME) ₂ four-membered ring (Cp = C ₅ H ₅ ; M = Ni, Pd, Pt; E = O, S, Se, Te). <i>New Journal of Chemistry</i> , 2017, 41, 12028-12034.	2.8	3

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109	Stability and donor-acceptor bond in dinuclear organometallics CpM1 μ -M2Cl3 (M1, M2 = B, Al, Ga, In; Cp = η^5 -C ₅ H ₅) Tj BCC	1.8	3
110	Regular/abnormal variation in the strength and nature of the halogen bond between H ₂ Te and the dihalogens: Prominent effect of methyl substituents. Applied Organometallic Chemistry, 2020, 34, e5468.	3.5	3
111	Interactions in Model Ionic Dyads and Triads Containing Tetrel Atoms. Molecules, 2020, 25, 4197.	3.8	3
112	Comparison for Electron Donor Capability of Carbon-Bound Halogens in Tetrel Bonds. ACS Omega, 2021, 6, 29037-29044.	3.5	3
113	Promotion of TH3 (T = Si and Ge) group transfer within a tetrel bond by a cation π interaction. Physical Chemistry Chemical Physics, 2022, 24, 1113-1119.	2.8	3
114	<i>ab initio</i> study of the structure, cooperativity, and vibrational properties of HNC ternary complexes with two HF molecules. Molecular Physics, 2009, 107, 1649-1654.	1.7	2
115	Synergistic and diminutive effects between halogen bond and lithium bond in complexes involving aromatic compounds. Journal of Molecular Modeling, 2015, 21, 257.	1.8	2
116	The addition reactions of germylenoid H ₂ GeAlCl ₃ with ethylene: a theoretical investigation. Journal of Molecular Modeling, 2017, 23, 199.	1.8	2
117	Halogen bond between hypervalent halogens YF ₃ /YF ₅ (Y=Cl, Br, I) and H ₂ X (X= O, S, Se). Molecular Physics, 2020, 118, e1656834.	1.7	2
118	Graphitic SiC : A potential anode material for Na-ion battery with extremely high storage capacity. International Journal of Quantum Chemistry, 2021, 121, e26608.	2.0	2
119	Fabricating Flexible Packaging Batteries in General Chemistry Laboratories. Journal of Chemical Education, 2021, 98, 2471-2475.	2.3	2
120	Noncovalent bond between tetrel π -hole and hydride. Physical Chemistry Chemical Physics, 2021, 23, 10536-10544.	2.8	2
121	Strong effect of methyl group on the strength of ionic hydrogen bond between C ₂ H ₂ and H ₃ O ⁺ . International Journal of Quantum Chemistry, 2009, 109, 870-875.	2.0	1
122	Comparative study of XO π -ClF and XS π -ClF (X = H, CH ₃ , and F) halogen π -bonded complexes. International Journal of Quantum Chemistry, 2011, 111, 3856-3863.	2.0	1
123	Effect of metal cations [Li ⁺ , Na ⁺ , K ⁺ , Be ²⁺ , Mg ²⁺ , and Ca ²⁺] on the structure of 2 π -(3-hydroxy-2-pyridyl)benzoxazole: A theoretical investigation. International Journal of Quantum Chemistry, 2013, 113, 1316-1324.		1
124	Influence of substituents and cooperativity in doubly hydrogen-bonded complexes of 2-pyridone and oxalic acid. Molecular Physics, 2018, 116, 1862-1870.	1.7	1
125	Theoretical assessing on the coordination mode and bonding in heteronuclear group π 3 dimetallocene. International Journal of Quantum Chemistry, 2018, 118, e25461.	2.0	1
126	Comparative study of 1:1 Lewis acid π -base adducts between Cp ₂ M(L)H (M = V, Nb, Ta; L = CO, C ₂ H ₄ , P(CH ₃) ₃) and BF ₃ /AlF ₃ . Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1

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127	Regulating PdC3/PtC3- π -thiophene interaction by small molecule doping (AgOTf, CuBr, CuI, CuBr ₂) Tj ETQq1 1 0.784314 1rgBT /Over	2.0	1
128	Noncovalent Interactions in Complexes Involving the Cyclic C ₂ H ₂ X (X=O, S, Se) Molecules and the Lewis Acids YF (Y=F, Cl, Br, H). ChemistrySelect, 2019, 4, 9506-9515.	1.5	1
129	New insights into the dihydrogen bonds (MH ⁺ ...H-X) in CpM(PMe ₃)(L)2H ₂ HX (M=Cr, Mo, W; L=PMe ₃ , CO;) Tj ETQq1 1 0	2.0	1
130	Can metal halides be electron donors in π -hole and π -hole tetrel bonds? Cooperativity with an alkaline-earth bond. International Journal of Quantum Chemistry, 2021, 121, e26771.	2.0	1
131	The role of nitro group on the excited-state relaxation mechanism of P-Z base pair. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 267, 120549.	3.9	1