Complementarity of QTAIM and MO theory in the study complexes

Coordination Chemistry Reviews 249, 633-662 DOI: 10.1016/j.ccr.2004.08.022

Citation Report

#	Article	IF	CITATIONS
5	ls there a Co–Co bond path in Co2(CO)6(μ-CO)(μ-C4H2O2)?. Chemical Physics Letters, 2005, 414, 122-126	. 1.2	14
6	Ultrafast Electron Diffraction: Dynamical Structures on Complex Energy Landscapes. ChemPhysChem, 2005, 6, 2228-2250.	1.0	27
7	Properties of interatomic surfaces: Relation to bond energies. Physical Chemistry Chemical Physics, 2005, 7, 3805.	1.3	5
8	Experimental X-ray Charge Density Studies on the Binary Carbonyls Cr(CO)6, Fe(CO)5, and Ni(CO)4. Journal of Physical Chemistry A, 2005, 109, 8834-8848.	1.1	73
9	Electron Density Distributions Calculated for the Nickel Sulfides Millerite, Vaesite, and Heazlewoodite and Nickel Metal:Â A Case for the Importance of Niâ^'Ni Bond Paths for Electron Transport. Journal of Physical Chemistry B, 2005, 109, 21788-21795.	1.2	41
10	Description of Electron Delocalization via the Analysis of Molecular Fields. Chemical Reviews, 2005, 105, 3812-3841.	23.0	160
11	Hydrogen–Hydrogen Bonding: The Non-Electrostatic Limit of Closed-Shell Interaction Between Two Hydro. , 2006, , 337-375.		66
12	Sodium compounds of the benzophenone dianion (diphenyloxidomethanide). Dalton Transactions, 2006, , 129-136.	1.6	21
13	Ab initio charge density analysis of (B6C)2– and B4C3 species – How to describe the bonding pattern?. Canadian Journal of Chemistry, 2006, 84, 771-781.	0.6	18
14	Extension of the Experimental Electron Density Analysis to Metastable States:Â A Case Example of the Spin Crossover Complex Fe(btr)2(NCS)2·H2O. Journal of the American Chemical Society, 2006, 128, 13921-13931.	6.6	47
15	Spatial Shape of Electron Delocalization:  Structure of the Laplacian of the Negative Exchangeâ~'Correlation Density. Journal of Physical Chemistry A, 2006, 110, 9273-9281.	1.1	13
16	A Comprehensive Theoretical View of the Bonding in Actinide Molecular Complexes. Journal of the American Chemical Society, 2006, 128, 2190-2191.	6.6	76
17	Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198.	1.2	39
18	Bond Length and Local Energy Density Property Connections for Non-Transition-Metal Oxide-Bonded Interactions. Journal of Physical Chemistry A, 2006, 110, 12259-12266.	1.1	33
19	Comparative Static and Dynamic Study of a Prototype SN2 Reaction. Journal of Chemical Theory and Computation, 2006, 2, 1220-1227.	2.3	24
20	Binding Energies of First Row Diatomics in the Light of the Interacting Quantum Atoms Approach. Journal of Physical Chemistry A, 2006, 110, 12864-12869.	1.1	91
21	Experimental charge-density study on the nickel(II) coordination complex [Ni(H3 L)][NO3][PF6] [H3 L = N,N′,N′′-tris(2-hydroxy-3-methylbutyl)-1,4,7-triazacyclononane]: a reappraisal. Acta Crystallographica Section B: Structural Science, 2006, 62, 236-244.	1.8	20
22	Application of the allylboration reaction of terminal acetylenes with allyldihaloboranes for the preparation of capping agents for the synthesis of precursors of polymeric iron(II) clathrochelates. Russian Chemical Bulletin, 2006, 55, 1971-1981.	0.4	5

#	Article	IF	CITATIONS
23	Pauli Repulsions Exist Only in the Eye of the Beholder. Chemistry - A European Journal, 2006, 12, 2896-2901.	1.7	240
24	Comment on the Comparative Use of the Electron Density and Its Laplacian. Chemistry - A European Journal, 2006, 12, 7769-7772.	1.7	39
26	Electron density analysis of the layered antiferromagnetic compoundCu2(OH)3NO3: Relationship with the magnetic interaction mechanism. Physical Review B, 2006, 73, .	1.1	20
27	Accounting for the Differences in the Structures and Relative Energies of the Highly Homoatomic npl̈€âr'npl̈€ (n ≥ 3)-Bonded S2I42+, the Seâr'l l̃€-Bonded Se2I42+, and Their Higher-Energy Isomers by AIM, Mu NBO, and VB Methodologies. Inorganic Chemistry, 2007, 46, 681-699.	0,1.9	19
28	Source function description of metal–metal bonding in d-block organometallic compounds. Faraday Discussions, 2007, 135, 55-78.	1.6	127
29	Forces in molecules. Faraday Discussions, 2007, 135, 79-95.	1.6	57
31	Interactions Involving Metals– From"Chemical Categories―to QTAIM, and Backwards. , 0, , 343-374.		6
32	Chemical bonding: From Lewis to atoms in molecules. Journal of Computational Chemistry, 2007, 28, 4-14.	1.5	85
33	Unicorns in the world of chemical bonding models. Journal of Computational Chemistry, 2007, 28, 15-24.	1.5	198
34	Electronic reorganization: Origin of sigma trans promotion effect. Journal of Computational Chemistry, 2007, 28, 423-441.	1.5	10
35	Self-aggregation of bilayer ferrocenyl termini gold nanoparticles. Inorganic Chemistry Communication, 2007, 10, 511-513.	1.8	4
36	Influence of weak coordination on the electronic characteristics of the copper(II) atom: charge density analysis in the crystal of azurite. Mendeleev Communications, 2007, 17, 71-73.	0.6	8
37	Letter to the Editor: The concept of chemical bond – some like it fuzzy but others concrete. Foundations of Chemistry, 2007, 9, 85-95.	0.4	10
38	Application of quantum theory of atoms in molecules on small single wall (6,0) zigzag carbon clusters. Part I: Topological analysis of electron density, structure and bonding. Computational and Theoretical Chemistry, 2008, 856, 79-87.	1.5	3
39	Electrostatic properties of small molecules by means of atomic multipoles from the quantum theory of atoms in molecules. International Journal of Quantum Chemistry, 2008, 108, 2417-2427.	1.0	10
40	Chemical Bonding in the Inclusion Complex of He in Adamantane (He@adam): The Origin of the Barrier to Dissociation. Chemistry - A European Journal, 2008, 14, 10223-10226.	1.7	58
41	Hydrogen-bonding interactions in monomeric dimethylcuprates. A theoretical study. Computational and Theoretical Chemistry, 2008, 861, 85-96.	1.5	3
42	Role of Inner- and Outer-Sphere Bonding in the Sensitization of Eu ^{III} -Luminescence Deciphered by Combined Analysis of Experimental Electron Density Distribution Function and Photophysical Data. Inorganic Chemistry, 2008, 47, 11095-11107.	1.9	159

#	ARTICLE	IF	CITATIONS
43	A Computational Study on Some Viable Targets for Gas-Phase Synthesis of Metal Complexes of the Cyclic (B ₆ C) ^{â^'2} and Their Bonding Pattern. Journal of Physical Chemistry A, 2008, 112, 10365-10377.	1.1	13
44	Localized-orbital locator (LOL) profiles of chemical bonding. Canadian Journal of Chemistry, 2008, 86, 695-702.	0.6	271
45	A Combined Experimental and Theoretical Charge Density Study of the Chemical Bonding and Magnetism in 3-Amino-propanolato Cu(II) Complexes Containing Weakly Coordinated Anions. Journal of Physical Chemistry A, 2008, 112, 9050-9067.	1.1	50
46	Nearsightedness of Electronic Matter As Seen by a Physicist and a Chemist. Journal of Physical Chemistry A, 2008, 112, 13717-13728.	1.1	39
47	Hindered Cluster Rotation and ⁴⁵ Sc Hyperfine Splitting Constant in Distonoid Anion Radical Sc ₃ N@C ₈₀ ^{â^'} , and Spatial Spinâ^'Charge Separation as a General Principle for Anions of Endohedral Fullerenes with Metal-Localized Lowest Unoccupied Molecular Orbitals. Journal of the American Chemical Society, 2008, 130, 17726-17742.	6.6	104
48	Pericyclic versus Pseudopericyclic Reactions. What the Laplacian of the Charge Density, â^‡ ² ï(<i>r</i>), Has To Say about It? The Case of Cycloaddition Reactions. Journal of Physical Chemistry A, 2008, 112, 8164-8178.	1.1	22
49	Experimental Bond Critical Point and Local Energy Density Properties Determined for Mna [®] O, Fea [®] O, and Coâ ^{°°} O Bonded Interactions for Tephroite, Mn2SiO4, Fayalite, Fe2SiO4, and Co2SiO4 Olivine and Selected Organic Metal Complexes: Comparison with Properties Calculated for Non-Transition and Transition Metal Mâ ^{°°} O Bonded Interactions for Silicates and Oxides. Journal of Physical Chemistry A, 2008, 112,	1.1	35
50	Estimation of Dissociation Energy in Donorâ [°] Acceptor Complex AuCl·PPh ₃ via Topological Analysis of the Experimental Electron Density Distribution Function. Journal of Physical Chemistry A, 2008, 112, 11519-11522.	1.1	97
51	Engineering delocalizing π electronic [Cull3(μ3-OH)(μ-pz)3]2+ species into organometallic frameworks by Ag-l€ coordination. CrystEngComm, 2008, 10, 1467.	1.3	18
52	Crucial role of Ruâ√H interactions in the crystal packing of ruthenocene and its derivatives. CrystEngComm, 2008, 10, 827.	1.3	40
53	Quantifying the Donorâ `Acceptor Properties of Carbon Monoxide and Its <i>Carbo</i> -mer Using ELF Analysis. Organometallics, 2008, 27, 5263-5272.	1.1	13
54	Role of Short-Range Electrostatics in Torsional Potentials. Journal of Physical Chemistry A, 2008, 112, 12954-12965.	1.1	33
55	QTAIM Analysis of Ligand Properties and Mechanisms of Tuning of 6-Membered Ring <i>N</i> -Heterocyclic Carbenes in Transition Metal Complexes through Ring-Substituent Variation. Journal of Physical Chemistry A, 2009, 113, 8647-8653.	1.1	4
57	Bonding in Endohedral Metallofullerenes as Studied by Quantum Theory of Atoms in Molecules. Chemistry - A European Journal, 2009, 15, 9707-9729.	1.7	155
58	Chemical bonding in view of electron charge density and kinetic energy density descriptors. Journal of Computational Chemistry, 2009, 30, 1093-1102.	1.5	62
59	A localized picture of back bonding in CH3â~'nXn (X=F, Cl and Br; n=1, 2 or 3) radical and cation systems. Computational and Theoretical Chemistry, 2009, 901, 96-102.	1.5	2
60	Chemical bonding in the lightest tri-atomic clusters; H3+, Li3+ and B3â^². Computational and Theoretical Chemistry, 2009, 901, 243-248.	1.5	19
61	Quantitative estimates of transferability of the QTAIM descriptors. Case study of the substituted hydropyrimidines. Computational and Theoretical Chemistry, 2009, 906, 11-24.	1.5	24

#	Article	IF	CITATIONS
62	The role of electronic delocalization in transition metal complexes from the electron localization function and the quantum theory of atoms in molecules viewpoints. Coordination Chemistry Reviews, 2009, 253, 647-665.	9.5	141
63	Multiple Bonding in the Chromium Dimer Supported by Two Diazadiene Ligands. Journal of Physical Chemistry A, 2009, 113, 1559-1563.	1.1	13
64	High- and Low-Temperature Modifications of Sc3RuC4 and Sc3OsC4—Relativistic Effects, Structure, and Chemical Bonding. Inorganic Chemistry, 2009, 48, 6436-6451.	1.9	31
65	DFT/TDDFT Exploration of the Potential Energy Surfaces of the Ground State and Excited States of Fe ₂ (S ₂ C ₃ H ₆)(CO) ₆ : A Simple Functional Model of the [FeFe] Hydrogenase Active Site. Journal of Physical Chemistry A, 2009, 113, 5657-5670.	1.1	30
66	A Density Functional Theory Study of the Topology of the Charge Density of Complexes of 8-Hydroxyquinoline with Mn(III), Fe(III), and Co(III). Journal of Physical Chemistry A, 2009, 113, 5205-5211.	1.1	6
67	Mutual Influence of Cyclopentadienyl and Carbonyl Ligands in Cymantrene: QTAIM Study. Journal of Physical Chemistry A, 2009, 113, 10845-10851.	1.1	30
69	Bond Paths Are Not Chemical Bonds. Journal of Physical Chemistry A, 2009, 113, 10391-10396.	1.1	544
70	Combined Experimental and Theoretical Study of (Î- ⁵ -C ₅ H ₅)Mn(CO) ₃ , (Î- ⁶ -C ₆ H ₆)Cr(CO) ₃ , and	6.6	170
71	Journal of the American Chemical Society, 2009, 131, 1251-1268. Confined Atoms Treated as Open Quantum Systems. Advances in Quantum Chemistry, 2009, 57, 285-318.	0.4	17
72	Hyperconjugation versus back bonding in AH3â^'nXn species (A=Si and Ge; X=F, Cl and Br; and n=1, 2 and) Tj ETQ	2q1 1 0.78 1.5	34314 rgBT
73	Why is monoalkylation versus bis-alkylation of the Ni(II) complex of the Schiff base of (S)-N-(2-benzoylphenyl)-1-benzylpyrrolidine-2-carboxamide and glycine so selective? MP2 modelling and topological QTAIM analysis of chiral metallocomplex synthons of α-amino acids used for the preparation of radiopharmaceuticals for positron emission tomography. Journal of Radioanalytical	0.7	3
74	and Nuclear Chemistry, 2010, 286, 829-833. A new chromium (III) complex containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide, (NPyPzCa): Synthesis, molecular and crystal structure and theoretical electron density analysis. Solid State Sciences, 2010, 12, 1960-1965.	1.5	3
75	On the stability of metal–aminoacid complexes in water based on water–ligand exchange reactions and electronic properties: Detailed study on iron–glycine hexacoordinated complexes. Journal of Computational Chemistry, 2010, 31, 2735-2745.	1.5	7
76	Topological study of bis(cyclopentadienyl) titanium and bent titanocenes. Chemical Physics Letters, 2010, 499, 193-198.	1.2	16
77	Metalâ^'Metal and Metalâ^'Ligand Bonding at a QTAIM Catastrophe: A Combined Experimental and Theoretical Charge Density Study on the Alkylidyne Cluster Fe ₃ (μ-H)(μ-COMe)(CO) ₁₀ . Journal of Physical Chemistry A, 2010, 114, 13418-1343	1.1 3.	91
78	Topological Characterization of the Electron Density Laplacian in Crystals. The Case of the Group IV Elements. Journal of Chemical Theory and Computation, 2010, 6, 3761-3779.	2.3	42
79	Investigating the Nature of Noble Gasâ^'Copper Bonds by the Quantum Theory of Atoms in Molecules. Journal of Physical Chemistry A, 2010, 114, 5222-5229.	1.1	15
80	Definition of Molecular Structure: By Choice or by Appeal to Observation?. Journal of Physical	1.1	176

#	Article	IF	CITATIONS
81	Preparation, structure and analysis of the bonding in the molecular entity (OSO)2Li{[AlF(ORF)3]Li[Al(ORF)4]} (RF = C(CF3)3). Dalton Transactions, 2010, 39, 2587.	1.6	13
82	Probing Mesitylborane and Mesitylborate Ligation Within the Coordination Sphere of Cp*Ru(P ^{<i>i</i>} Pr ₃) ⁺ : A Combined Synthetic, X-ray Crystallographic, and Computational Study. Inorganic Chemistry, 2011, 50, 2431-2444.	1.9	45
83	Iron(0) Promotes Aza Cyclization of an Elusive Ferrocenylketene. Organometallics, 2011, 30, 4830-4837.	1.1	13
84	Worlds Apart in Chemistry: A Personal Tribute to J. C. Slater. Journal of Physical Chemistry A, 2011, 115, 12667-12676.	1.1	28
85	Chemical Information from Charge Density Studies. , 2011, , 435-467.		0
86	Interatomic Magnetizability: A QTAIM-Based Approach toward Deciphering Magnetic Aromaticity. Journal of Physical Chemistry A, 2011, 115, 12555-12560.	1.1	35
87	Theoretical Insights into the Nature of Nickelâ^'Carbon Dioxide Interactions in Ni(PH ₃) ₂ (η ² -CO ₂). Journal of Physical Chemistry A, 2011, 115, 12463-12473.	1.1	20
88	Valence Shell Charge Concentration (VSCC) Evolution: A Tool to Investigate the Transformations within a VSCC Throughout a Chemical Reaction. Journal of Physical Chemistry A, 2011, 115, 12924-12932.	1.1	14
89	Intramolecular Hypervalent Interaction in the Conjugate Five-Membered Rings. Journal of Physical Chemistry A, 2011, 115, 12973-12982.	1.1	13
90	List of Publications for Richard F. W. Bader. Journal of Physical Chemistry A, 2011, 115, 12438-12444.	1.1	3
91	Subshell Fitting of Relativistic Atomic Core Electron Densities for Use in QTAIM Analyses of ECP-Based Wave Functions. Journal of Physical Chemistry A, 2011, 115, 12879-12894.	1.1	41
92	Relativistic-Consistent Electron Densities of the Coinage Metal Clusters M ₂ , M ₄ , M ₄ ^{2–} , and M ₄ Na ₂ (M = Cu, Ag, Au): A QTAIM Study. Journal of Physical Chemistry A, 2011, 115, 13024-13035.	1.1	19
93	Linear Response and Measures of Electron Delocalization in Molecules. Current Organic Chemistry, 2011, 15, 3609-3618.	0.9	18
94	Application of Electron Delocalization Indicators in the Study of Electrophilic Aromatic Substitution Reactions. Current Organic Chemistry, 2011, 15, 3627-3651.	0.9	5
96	Beyond the bond. Nature, 2011, 469, 26-28.	13.7	61
97	On the non-existence of parallel universes in chemistry. Foundations of Chemistry, 2011, 13, 11-37.	0.4	49
98	Molecular structure of cyanidin metal complexes: Al(III) versus Mg(II). Theoretical Chemistry Accounts, 2011, 128, 485-495.	0.5	18
99	Molecular Structure and Antimicrobial Activity of a Luminescent Dinuclear Silver(I) Complex of Phenylâ€bis(2â€pyridyl)phosphine. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 2260-2264.	0.6	9

#	Article	IF	CITATIONS
100	The quantum divided basins: A new class of quantum subsystems. International Journal of Quantum Chemistry, 2011, 111, 2788-2801.	1.0	32
101	A Theoretical Study of the 3dâ€M(smif) ₂ Complexes: Structure, Magnetism, and Oxidation States. ChemPhysChem, 2011, 12, 3236-3244.	1.0	7
102	Chemical bonding in complexes with high coordination numbers: a charge density study. Mendeleev Communications, 2011, 21, 160-162.	0.6	14
103	The critical re-evaluation of the aromatic/antiaromatic nature of Ti3(CO)3: a missed opportunity?. Physical Chemistry Chemical Physics, 2011, 13, 4576.	1.3	27
104	Dimethylaminoborane (H ₂ BNMe ₂) Coordination to Late Transition Metal Centers: Snapshots of the B–H Oxidative Addition Process Inorganic Chemistry, 2011, 50, 11039-11045.	1.9	49
105	Molecular recognition between DNA and a copper-based anticancer complex. Physical Chemistry Chemical Physics, 2012, 14, 15539.	1.3	55
106	Can a Single Molecule of Water be Completely Isolated Within the Subnanoâ€6pace Inside the Fullerene C ₆₀ Cage? A Quantum Chemical Prospective. Chemistry - A European Journal, 2012, 18, 15345-15360.	1.7	44
107	Conformational preference of 2,5-disubstituted phosphacymantrenes evidenced by the data of quantum chemical calculations and topology analysis of electron density. Russian Chemical Bulletin, 2012, 61, 2204-2211.	0.4	8
108	Advances in Understanding of Chemical Bonding: Inputs from Experimental and Theoretical Charge Density Analysis. Journal of Physical Chemistry A, 2012, 116, 9791-9801.	1.1	43
109	Hydrogen-Bonding Interactions and Properties of Energetic Nitroamino[1,3,5]triazine-Based Guanidinium Salts: DFT-D and QTAIM Studies. Chemistry - an Asian Journal, 2012, 7, 2577-2591.	1.7	18
110	QTAIM Analysis of the Bonding in Mo–Mo Bonded Dimolybdenum Complexes. Inorganic Chemistry, 2012, 51, 7384-7391.	1.9	21
111	QTAIM View of Metal–Metal Bonding in Di- and Trinuclear Disulfido Carbonyl Clusters. Organometallics, 2012, 31, 2559-2570.	1.1	46
112	Theoretical study of the smiles rearrangement in the activation mechanism of proton pump inhibitors. Journal of Physical Organic Chemistry, 2012, 25, 230-238.	0.9	5
113	Bonding between strongly repulsive metal atoms: an oxymoron made real in a confined space of endohedral metallofullerenes. Chemical Communications, 2012, 48, 8031.	2.2	99
114	A Bond Path and an Attractive Ehrenfest Force Do Not Necessarily Indicate Bonding Interactions: Case Study on M ₂ X ₂ (M=Li, Na, K; X=H, OH, F, Cl). Chemistry - A European Journal, 2012, 18, 4982-4993.	1.7	72
115	Structures and Stability of Fullerenes, Metallofullerenes, and Their Derivatives. , 2012, , 667-721.		0
116	Al42â^'; the anion–π interactions and aromaticity in the presence of counter ions. Physical Chemistry Chemical Physics, 2012, 14, 9738.	1.3	11
117	Peculiarities of the M–Ĩ€ interaction in phosphacymantrene derivatives upon the Mn(CO)3 fragment orientation: Experimental and theoretical electron density study. Journal of Molecular Structure, 2012, 1014, 81-91.	1.8	12

#	Article	IF	CITATIONS
118	Nature of the ringâ€closure process along the rearrangement of octaâ€1,3,5,7â€tetraene to cyclooctaâ€1,3,5â€triene from the perspective of the electron localization function and catastrophe theory. Journal of Computational Chemistry, 2012, 33, 748-756.	1.5	44
119	Relation between topology and stability of bent titanocenes. Journal of Molecular Modeling, 2013, 19, 2955-2964.	0.8	3
120	Electron Density Analysis. , 2013, , 187-226.		21
121	CO-Induced Methyl Migration in a Rhodium Thiophosphoryl Pincer Complex and Its Comparison with Phosphine-Based Complexes: The Divergent Effects of S and P Donor Ligands. Organometallics, 2013, 32, 7163-7180.	1.1	18
122	Hydrogenâ€Bond Cooperative Effects in Small Cyclic Water Clusters as Revealed by the Interacting Quantum Atoms Approach. Chemistry - A European Journal, 2013, 19, 14304-14315.	1.7	80
123	Experimental QTAIM Analysis of the Electron Density in TiB ₂ . Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 2065-2070.	0.6	7
124	Extremely Long Cu··A·O Contact as a Possible Pathway for Magnetic Interactions in Na ₂ Cu(CO ₃) ₂ . Inorganic Chemistry, 2013, 52, 14355-14363.	1.9	15
125	Studies of the Structures and Bonding of Gold-Bridged Dirhenium Carbonyl Cluster Complexes. Organometallics, 2013, 32, 7540-7546.	1.1	9
126	Quantifying the Nature of Lone Pair Domains. ChemPhysChem, 2013, 14, 3714-3725.	1.0	28
127	Electronic structure of [Ni(II)S4] complexes from S K-edge X-ray absorption spectroscopy. Coordination Chemistry Reviews, 2013, 257, 564-578.	9.5	33
128	Structure, energy, vibrational spectrum, and Bader's analysis of π⋯H hydrogen bonds and H ^{â~δ} â<¯H ^{+δ} dihydrogen bonds. Physical Chemistry Chemical Physics, 2013, 15, 37-79.	1.3	63
129	Di- and Triphenylacetates of Lanthanum and Neodymium. Synthesis, Structural Diversity, and Application in Diene Polymerization. Organometallics, 2013, 32, 1272-1286.	1.1	39
130	An efficient method for computing the QTAIM topology of a scalar field: The electron density case. Journal of Computational Chemistry, 2013, 34, 681-686.	1.5	79
131	On the Electronic Structure of <i>mer</i> , <i>trans</i> â€{RuCl ₃ (1 <i>H</i> â€indazole) ₂ (NO)], a Hypothetical Metabolite of the Antitumor Drug Candidate KP1019: An Experimental and DFT Study. European Journal of Inorganic Chemistry, 2013, 2013, 2505-2519.	1.0	18
132	Endohedral Fullerenes. Chemical Reviews, 2013, 113, 5989-6113.	23.0	1,103
133	A theoretical survey on the D7d [84]fullerene, a fullerene with two heptagon rings. Computational and Theoretical Chemistry, 2013, 1009, 103-107.	1.1	5
134	Deprotonation of <i>C</i> â€Alkyl Groups of Cationic Triruthenium Clusters Containing Cyclometalated <i>C</i> â€Alkylpyrazinium Ligands: Experimental and Computational Studies. Chemistry - A European Journal, 2013, 19, 9251-9260.	1.7	10
135	Forced Bonding and QTAIM Deficiencies: A Case Study of the Nature of Interactions in He@Adamantane and the Origin of the High Metastability. Chemistry - A European Journal, 2013, 19, 10945-10957.	1.7	22

ARTICLE IF CITATIONS The two-component quantum theory of atoms in molecules (TC-QTAIM): tensor formulation and its 136 0.5 18 implications. Theoretical Chemistry Accounts, 2013, 132, 1. Chemical Bond Characterization of a Mixed-Valence Tri-Cobalt Complex, Co₃(μ-admtrz)₄(μ-OH)₂(CN)₆Â2H₂O. Inorganic Chemistry, 2013, 52, 11023-11033. Computational Studies of Endohedral Fullerenes: Bonding, Isomerism, Internal Dynamics, 138 0 Spectroscopy, and Chemical Reactivity., 2014, , 315-399. Quantum Chemical Determination of Novel C₈₂ Monometallofullerenes Involving a Heterogeneous Group. Inorganic Chemistry, 2014, 53, 12911-12917. Laplacian of the electron density: a hole–lump interaction as a tool to study stereoelectronic 140 0.9 7 control of chemical reactions. Journal of Physical Organic Chemistry, 2014, 27, 327-335. DFT assessment of the spectroscopic constants and absorption spectra of neutral and charged diatomic species of group 11 and 14 elements. Journal of Computational Chemistry, 2014, 35, 1762-1777. 1.5 The πâ€Backâ€Bonding Modulation and Its Impact in the Electronic Properties of Cu^{II} 142 Antineoplastic Compounds: An Experimental and Theoretical Study. Chemistry - A European Journal, 1.7 35 2014, 20, 13730-13741. Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. International 84 Journal of Quantum Chemistry, 2014, 114, 1239-1252. Properties of atoms in electronically excited molecules within the formalism of TDDFT. Journal of 145 1.5 22 Computational Chemistry, 2014, 35, 820-828. 146 Dynamic Molecular Graphs: "Hopping―Structures. Chemistry - A European Journal, 2014, 20, 5665-5672. 1.7 On the structure of Zn(II) and Cu(II) cyanin complexes in aqueous solution. Structural Chemistry, 147 2 1.0 2014, 25, 1647-1657. Metal- and Ligand-Supported Reduction of the {Fe₂S₂} Cluster as a Path to Formation of Molecular Group 13 Element Complexes {Fe₂S₂M} (M = Al, Ga). Organometallics, 2014, 33, 2713-2720. 1.1 Topological reaction sites – very strong chalcogen bonds. Physical Chemistry Chemical Physics, 2014, 149 1.3 97 16, 2430-2442. Potential energy surface and binding energy in the presence of an external electric field: modulation of anion–Ĩ€ interactions for graphene-based receptors. Physical Chemistry Chemical Physics, 2014, 16, 1.3 2508-2514. Effects of Axial Coordination on Immobilized Mn(salen) Catalysts. Journal of Physical Chemistry A, 151 1.1 10 2014, 118, 10788-10796. Computational Study on Cycloisomerization/Oxidative Dimerization of Aryl Propargyl Ethers 14 Catalyzed by Gold Nanoclusters: Mechanism and Selectivity. Organometallics, 2014, 33, 6633-6642. Trinuclear alkyl hydrido rare-earth complexes supported by amidopyridinato ligands: synthesis, structures, C–Śi bond activation and catalytic activity in ethylene polymerization. Dalton 153 1.6 12 Transactions, 2014, 43, 14450-14460. Sc₂S@C₆₈: an obtuse di-scandium sulfide cluster trapped in a C_{2v} 154 1.3 fullerene cage. Physical Chemistry Chemical Physics, 2014, 16, 15994-16002.

#	Article	IF	Citations
155	Convergent study of Ru–ligand interactions through QTAIM, ELF, NBO molecular descriptors and TDDFT analysis of organometallic dyes. Molecular Physics, 2014, 112, 2063-2077.	0.8	9
156	The stability of B15N15Hx nano-rings is affected by electron delocalization. Computational and Theoretical Chemistry, 2014, 1046, 1-5.	1.1	4
157	On the regioselectivity of the mononuclear copper-catalyzed cycloaddition of azide and alkynes (CuAAC). A quantum chemical topological study. Journal of Molecular Modeling, 2014, 20, 2187.	0.8	13
158	Toward a Consistent Interpretation of the QTAIM: Tortuous Link between Chemical Bonds, Interactions, and Bond/Line Paths. Chemistry - A European Journal, 2014, 20, 10140-10152.	1.7	194
159	Picture change error in quasirelativistic electron/spin density, Laplacian and bond critical points. Chemical Physics, 2014, 438, 37-47.	0.9	14
160	The Nâ <l 144-148.<="" 2014,="" 601,="" and="" as="" bond="" by="" chemical="" delocalization="" function="" halogen="" in="" indices.="" letters,="" physics="" pyridines="" source="" substituted="" td="" the="" viewed=""><td>1.2</td><td>29</td></l>	1.2	29
161	Facile cleavage of phenyl groups from BiPh3 in its reactions with Os3(CO)10(NCMe)2 and evidence for localization of ï€-bonding in a bridging benzyne ligand. Journal of Organometallic Chemistry, 2014, 751, 475-481.	0.8	10
162	Synthesis, X-ray investigation and DFT calculations of solvated barium Î ² -diketonate complexes with 18-dibenzocrown-6: [Ba(pta)2(18DBC6)](C6H5CH3)2 and [Ba(pta)2(18DBC6)](CH2Cl2) (pta=1,1,1-trifluoro-5,5-dimethylhexanedionato-2,4; 18DBC6=18-dibenzocrown-6). Polyhedron, 2014, 79, 229-238.	1.0	2
163	Origin of the Extra Stability of Alloxan. A Computation Study. Procedia Computer Science, 2014, 29, 1366-1375.	1.2	0
164	Saturated vs. unsaturated hydrocarbon interactions with carbon nanostructures. Frontiers in Chemistry, 2014, 2, 75.	1.8	6
165	Features of chemical bonding within the Fe(NO)2 fragment for crystalline bis(thiosulfate) tetranitrosyl diiron tetramethylammonium salt as an example according to high-resolution X-ray diffraction data. Russian Chemical Bulletin, 2015, 64, 2351-2360.	0.4	5
166	Syntheses of Ir4(CO)6(η5-C5Me4H)2and Ir7(μ43-CO)3(CO)12(η5-C5Me5) from Pentametallic Molybdenum-Iridium Cluster Precursors. European Journal of Inorganic Chemistry, 2015, 2015, 2587-2591.	1.0	2
167	Electron Density Analysis of Hyperconjugation. ChemPhysChem, 2015, 16, 3842-3845.	1.0	3
168	From Dibismuthenes to Three―and Twoâ€Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC ₃ N Rings through a Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2015, 21, 16917-16928.	1.7	76
169	Ferrocene Orientation Determined Intramolecular Interactions Using Energy Decomposition Analysis. Materials, 2015, 8, 7723-7737.	1.3	13
170	From Stiba- and Bismaheteroboroxines to N,C,N-Chelated Diorganoantimony(III) and Bismuth(III) Cations—An Unexpected Case of Aryl Group Migration. Inorganic Chemistry, 2015, 54, 6010-6019.	1.9	20
171	Sequential metalation of benzene: electronic, bonding, magnetotropic and spectroscopic properties of coinage metalated benzenes studied by DFT. Journal of Molecular Modeling, 2015, 21, 153.	0.8	6
172	Homopolar dihydrogen bonding in main group hydrides: discovery, consequences, and applications. Dalton Transactions, 2015, 44, 9718-9731.	1.6	48

#	Article	IF	CITATIONS
173	On the transferability of electron density in binary vanadium borides VB, V ₃ B ₄ and VB ₂ . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 777-787.	0.5	4
174	Where to place the positive muon in the Periodic Table?. Physical Chemistry Chemical Physics, 2015, 17, 7023-7037.	1.3	23
175	Rationalizing the Catalytic Activity of Copper in the Cycloaddition of Azide and Alkynes (CuAAC) with the Topology of â^‡ ² i(<i></i>) and â^‡â^‡ ² i(<i></i>). Journal of Physical Chemistry B, 2015, 119, 1243-1258.	1.2	28
176	Asymmetric bifurcated halogen bonds. Physical Chemistry Chemical Physics, 2015, 17, 6440-6450.	1.3	58
177	The d-electrons of Fe in ferrocene: the excess orbital energy spectrum (EOES). RSC Advances, 2015, 5, 11933-11941.	1.7	16
178	Lewis-acid induced disaggregation of dimeric arylantimony oxides. Chemical Communications, 2015, 51, 5932-5935.	2.2	27
179	Understanding the Electronic Factors Responsible for Ligand Spin–Orbit NMR Shielding in Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1509-1517.	2.3	54
180	The Addition of Gold and Tin to Bismuth–Triiridium Carbonyl Complexes. Inorganic Chemistry, 2015, 54, 8042-8048.	1.9	10
181	Sterically Congested 5-Diphenylphosphinoacenaphth-6-yl-silanes and -silanols. Organometallics, 2015, 34, 3873-3887.	1.1	21
182	The hydrogen storage capacity of coinage metalated benzenes studied by DFT. Journal of Coordination Chemistry, 2015, 68, 2653-2665.	0.8	1
183	Towards Understanding the Decomposition/Isomerism Channels of Stratospheric Bromine Species: Ab Initio and Quantum Topology Study. International Journal of Molecular Sciences, 2015, 16, 6783-6800.	1.8	7
184	Electronic structure of kaempferol–Cu2+ coordination compounds: a DFT, QTAIM and NBO study in the gas phase. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	5
185	Toward understanding tautomeric switching in 4-hydroxynaphthaldehyde and its dimers: A DFT and quantum topology study. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550016.	1.8	3
186	Molecular insight into the inhibition mechanism of plant and rat 4-hydroxyphenylpyruvate dioxygenase by molecular docking and DFT calculations. Medicinal Chemistry Research, 2015, 24, 3958-3971.	1.1	25
187	Multi-center covalency: revisiting the nature of anion–π interactions. Physical Chemistry Chemical Physics, 2015, 17, 30670-30679.	1.3	87
188	Guilty on Two Counts: Stepwise Coordination of Two Fluoride Anions to the Antimony Atom of a Noninnocent Stibine Ligand. Organometallics, 2015, 34, 2647-2654.	1.1	48
189	Unwilling U–U bonding in U ₂ @C ₈₀ : cage-driven metal–metal bonds in di-uranium fullerenes. Physical Chemistry Chemical Physics, 2015, 17, 24182-24192.	1.3	47
191	Electronic structure of alloxan and its dimers: QM/QD simulations and quantum chemical topology analysis. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2121-2132.	2.0	2

#	Article	IF	CITATIONS
192	QTAIM study of substituent effects on the intramolecular hydrogen bond in 3,3′-dihydroxy-4,4′-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. Journal of Molecular Structure, 2015, 1083, 1-9.	1.8	8
193	Chemical structure and reactivity by means of quantum chemical topology analysis. Computational and Theoretical Chemistry, 2015, 1053, 17-30.	1.1	62
194	The polarizability of organometallic bonds. Computational and Theoretical Chemistry, 2015, 1053, 165-172.	1.1	12
195	Relationship of QTAIM and NOCV Descriptors with Tolman's Electronic Parameter. Advances in Chemistry, 2016, 2016, 1-7.	1.1	3
196	Comparisons between Crystallography Data and Theoretical Parameters and the Formation of Intramolecular Hydrogen Bonds: Benznidazole. Crystals, 2016, 6, 56.	1.0	4
197	Experimental and theoretical characterization of Fe2Cr trinuclear-oxo-centered complex with a CF2ClCOO– bridge. Journal of Structural Chemistry, 2016, 57, 875-883.	0.3	1
198	Phosphanâ€stabilisierte Borylene und Borylâ€Anionen als Liganden? Redoxaktivitäin Borâ€basierten Pinzettenâ€Komplexen. Angewandte Chemie, 2016, 128, 14665-14670.	1.6	12
199	The barrier to the methyl rotation in <scp><i>C</i></scp> <i>is</i> â€2â€butene and its isomerization energy to <scp><i>T</i></scp> <i>rans</i> â€2â€butene, revisited. Journal of Computational Chemistry, 2016, 37, 143-154.	1.5	28
200	Germylenes and stannylenes stabilized within N ₂ PE rings (E = Ge or Sn): combined experimental and theoretical study. Dalton Transactions, 2016, 45, 10343-10354.	1.6	10
201	Phosphineâ€Stabilized Borylenes and Boryl Anions as Ligands? Redox Reactivity in Boronâ€Based Pincer Complexes. Angewandte Chemie - International Edition, 2016, 55, 14450-14454.	7.2	38
202	Electron density analysis of bent aromatic molecules: intramolecular interactions in small paracyclophanes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	4
203	Tracing the Fingerprint of Chemical Bonds within the Electron Densities of Hydrocarbons: A Comparative Analysis of the Optimized and the Promolecule Densities. ChemPhysChem, 2016, 17, 3260-3268.	1.0	12
205	Insight into structural and π–magnesium bonding characteristics of the X ₂ Mgâ‹ັY (X = H, F;) Tj E complexes. RSC Advances, 2016, 6, 102754-102761.	TQq0 0 0 r 1.7	gBT /Overloc 20
206	Noble Gas Binding Ability of Metalâ€Bipyridine Monocationic Complexes (Metal=Cu, Ag, Au): A Computational Study. ChemistrySelect, 2016, 1, 5842-5849.	0.7	18
207	Use of Quantum Theory of Atoms in Molecules in the Search for Appropriate Hydrogen Atom Locations in X-ray Diffraction Based Studies. Crystal Growth and Design, 2016, 16, 6841-6848.	1.4	8
208	Modulating Electron Sharing in Ion-ï€-Receptors via Substitution and External Electric Field: A Route toward Bond Strengthening. Journal of Chemical Theory and Computation, 2016, 12, 3788-3795.	2.3	42
209	Interactions in the ionic liquid [EMIM][FAP]: a coupled experimental and computational analysis. Physical Chemistry Chemical Physics, 2016, 18, 2617-2628.	1.3	25
210	Bonding in molecular crystals from the local electronic pressure viewpoint. Molecular Physics, 2016, 114, 1260-1269.	0.8	12

		EPORT	
#	Article	IF	CITATIONS
211	Unification of ground-state aromaticity criteria – structure, electron delocalization, and energy – in light of the quantum chemical topology. Physical Chemistry Chemical Physics, 2016, 18, 11693-11699.	1.3	72
212	How π back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes. Chemical Science, 2016, 7, 1174-1184.	3.7	158
213	Halogen bonding. The role of the polarizability of the electron-pair donor. Physical Chemistry Chemical Physics, 2016, 18, 7300-7309.	1.3	43
214	Multicenter transformations of the methyl ligand in CH3Os3Au carbonyl cluster complexes: Synthesis, characterization and DFT analyses. Journal of Organometallic Chemistry, 2016, 812, 95-107.	0.8	3
215	A topological analysis of the bonding in [M2(CO)10] and [M3(μ-H)3(CO)12] complexes (MÂ=ÂMn, Tc, Re). Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	25
216	Optimal wavelet signal compression as an efficient alternative to investigate molecular dynamics simulations: application to thermal and solvent effects of MRI probes. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	43
217	Stacking of dicarbonylacetylacetonatorhodium(I) molecules. Computational and Theoretical Chemistry, 2017, 1101, 30-35.	1.1	6
218	Structures and Stability of Fullerenes, Metallofullerenes, and Their Derivatives. , 2017, , 1031-1096.		0
219	A comparative DFT study of stacking interactions between adjacent metal atoms in linear chains of Ir and Rh acetylacetonato complexes. Journal of Organometallic Chemistry, 2017, 833, 88-94.	0.8	4
220	Evolution of electron density towards the conical intersection of a nucleic acid purine. Chemical Physics Letters, 2017, 683, 425-430.	1.2	7
221	Evolution of the interaction between C ₂₀ cage and Cr(CO) ₅ : A solvent effect, QTAIM and EDA investigation. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750007.	1.8	6
222	Performance of the RI and RIJCOSX approximations in the topological analysis of the electron density. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	6
223	Theoretical Investigation of the Binding of Nucleobases to Cucurbiturils by Dispersion Corrected DFT Approaches. Journal of Physical Chemistry B, 2017, 121, 4733-4744.	1.2	40
224	The Role of the DNA Backbone in Minorâ€Groove Ligand Binding. ChemPhysChem, 2017, 18, 1909-1915.	1.0	14
225	Rhodium-rhodium interactions in [Rh(β-diketonato)(CO)2] complexes. Journal of Molecular Structure, 2017, 1144, 280-289.	1.8	13
226	Delocalized and localized donating–accepting Mn–C interactions in half-sandwich cyclopentadienyl and pentadienyl complexes. Dalton Transactions, 2017, 46, 6958-6967.	1.6	7
227	Topological analysis of the metal-metal bond: A tutorial review. Coordination Chemistry Reviews, 2017, 345, 150-181.	9.5	108
228	Binding of Small Gas Molecules by Metal–Bipyridyl Monocationic Complexes (Metal = Cu, Ag, Au) and Possible Bond Activations Therein. Journal of Physical Chemistry A, 2017, 121, 3803-3817.	1.1	16

ARTICLE IF CITATIONS Structural and electronic features of triphenylstibine-functionalized Fischer carbene complexes of 229 1.0 10 molybdenum(0). Polyhedron, 2017, 133, 307-318. Time dependent – density functional theory characterization of organic dyes for dye-sensitized solar cells. Molecular Simulation, 2017, 43, 1523-1531. A Pseudohypervalent Sulfur Intermediate as an Oxidative Protective Mechanism in the Archaea 231 1.2 4 Peroxiredoxin Enzyme ApTPx. Journal of Physical Chemistry B, 2017, 121, 6570-6579. The Role of Ligand Steric Bulk in New Monovalent Aluminum Compounds. Journal of Physical 1.1 Chemistry A, 2017, 121, 4678-4687. Mechanistic investigation of cis and trans oxidative addition to 233 1.0 0 acetylacetonato-1,5-cyclooctadieneiridium(I). Polyhedron, 2017, 123, 252-258. Real-Space Bonding Indicator Analysis of the Donor–Acceptor Complexes X₃BNY₃, X₃AlNY₃, X₃, 3</sub>, 1.1 7717-7725 Packing polymorphism of dicarbonyl-[2-(phenylamino)pent-3-en-4-onato]rhodium(I). Journal of 235 0.8 6 Organometallic Chemistry, 2017, 851, 235-247. On understanding the chemical origin of band gaps. Journal of Molecular Modeling, 2017, 23, 271. 9 236 0.8 Facile activation of alkynes with a boraguanidinato-stabilized germylene: a combined experimental and 237 1.6 10 theoretical study. Dalton Transactions, 2017, 46, 12339-12353. Quantum Chemical Insight into La₂C₉₆: Metal Carbide Fullerene La₂C₂@C₉₄ versus Dimetallofullerene 1.9 La₂@C₉₆. Inorganic Chemistry, 2017, 56, 11883-11890. DFTâ€6upported Threshold Ionization Study of Chromium Biphenyl Complexes: Unveiling the Mechanisms of Substituent Influence on Redox Properties of Sandwich Compounds. Chemistry - A European 239 1.7 10 Journal, 2017, 23, 13669-13675. Investigation of Chemical Bonding in In Situ Cryocrystallized Organometallic Liquids. ChemPhysChem, 240 1.0 2017, 18, 2859-2863. Exploring the regioselectivity in the cycloaddition of azides to alkynes catalyzed by dinuclear copper clusters (Cu2AAC reaction) using the topologies of \hat{a}^{2} (r) and \hat{a}^{2} (r). Journal of Molecular Modeling, 241 0.8 6 2017, 23, 337. Linking the Character of the Metal–Ligand Bond to the Ligand NMR Shielding in Transition-Metal Complexes: NMR Contributions from Spin–Orbit Coupling. Journal of Chemical Theory and 242 2.3 Computation, 2017, 13, 3586-3601. Synthesis, experimental and theoretical characterization of a Mn(II) complex of 243 23 1.8 N,Nâ€²-dipyridoxyl(1,2-diaminobenzene). Journal of Molecular Structure, 2017, 1127, 15-22. Solvent effect on the linkage isomerism in [Fe(CO)₄(NCS)]^{â^'}and [Fe(CO)₄(SCŇ)]^{â^{*}}anions: A theoretical investigation. Physics and Chemistry of 244 Liquids, 2017, 55, 444-456. Variational quantum Monte Carlo results for N<sub>2, N_{2}^{+} and C_{2}^{a€"} 245 0.4 1 utilising the four-dimensional density of Bright Wilson. Physics and Chemistry of Liquids, 2017, 55, 281-290. 246 Intuitive Quantifiers of Charge Flows in Coordinate Bonding. Organometallics, 2017, 36, 3205-3214. 1.1 19

#	Article	IF	CITATIONS
247	Exploring EPR Parameters of ⁹⁹ Tc Complexes for Designing New MRI Probes: Coordination Environment, Solvent, and Thermal Effects on the Spectroscopic Properties. Journal of Chemistry, 2017, 2017, 1-8.	0.9	8
248	Insight into the thermodynamically preferred V3N@I(31924)-C80 and acknowledged VxSc3-xN@I(31924)-C80 (x=0, 1 and 2). Carbon, 2018, 132, 312-322.	5.4	9
249	Novel dichloro(bis{2-[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl-κN3]pyridine-κN})metal(II) coordination compounds of seven transition metals (Mn, Fe, Co, Ni, Cu, Zn and Cd). Polyhedron, 2018, 151, 243-254.	1.0	9
250	FALDIâ€based decomposition of an atomic interaction line leads to 3D representation of the multicenter nature of interactions. Journal of Computational Chemistry, 2018, 39, 973-985.	1.5	10
251	Why Bond Critical Points Are Not "Bond―Critical Points. Chemistry - A European Journal, 2018, 24, 5401-5405.	1.7	129
252	On the covalence in H2AuX (XÂ=ÂF–I). International Journal of Hydrogen Energy, 2018, 43, 1709-1717.	3.8	6
253	The influence of the negative hyperconjugation is relevant for the analysis of the π-π* conjugation with the mono-substitution and di-substitution of H2C= by O= and/or HN= in trans-buta-1,3-diene?. Structural Chemistry, 2018, 29, 847-857.	1.0	18
254	An experimental and DFT study of the packing and structure of dithenoylmethane monocarbonylphosphine Rhodium(I) complex [Rh((C 4 H 3 S)COCHCO(C 4 H 3 S))(CO)(PPh 3)]. Journal of Molecular Graphics and Modelling, 2018, 83, 33-41.	1.3	0
255	Analyzing Fluxional Molecules Using DORI. Journal of Chemical Theory and Computation, 2018, 14, 2370-2379.	2.3	5
256	The dizinc bond as a ligand: A computational study of elongated dizinc bonds. Inorganica Chimica Acta, 2018, 470, 197-205.	1.2	8
257	Noble gas encapsulated B ₄₀ cage. Physical Chemistry Chemical Physics, 2018, 20, 1953-1963.	1.3	41
258	DFT and CV data of 4-phenyl-substituted dichloro(bis{2-[1-(phenyl)-1H-1,2,3-triazol-4-yl-îºN3]pyridine-îºN})iron(II) coordination compounds. Data in Brief, 2018, 21, 1458-1471.	0.5	0
259	Theoretical Study of the Arene Ligand Effect on the Structure and Properties of Cr(CO)3(Arene) Complexes (Arene = Benzene, Biphenyl, Triphenly, Tetraphenyl). Journal of Structural Chemistry, 2018, 59, 1784-1790.	0.3	3
260	Theoretical Study of the Solvent Effect on the Electronic and Vibrational Properties of [CpFe(CO)2(NCS)] and [CpFe(CO)2(SCN)] Linkage Isomers. Journal of Structural Chemistry, 2018, 59, 1058-1066.	0.3	3
261	CAl ₃ X (X = B/Al/Ga/In/Tl) with 16 valence electrons: can planar tetracoordinate carbon be stable?. Physical Chemistry Chemical Physics, 2018, 20, 26266-26272.	1.3	22
262	A challenging redox neutral Cp*Co(III)-catalysed alkylation of acetanilides with 3-buten-2-one: synthesis and key insights into the mechanism through DFT calculations. Beilstein Journal of Organic Chemistry, 2018, 14, 2366-2374.	1.3	7
263	Behaviors and interactions of H2 absorption to CuRn+. International Journal of Hydrogen Energy, 2018, 43, 20892-20899.	3.8	3
264	Quantum chemical study of formation of Cull–YIII metallamacrocyclic complexes based on glycinehydroximate ligands. Russian Chemical Bulletin, 2018, 67, 1173-1181.	0.4	7

#	Article	IF	CITATIONS
265	First-principles and Molecular Dynamics simulation studies of functionalization of Au32 golden fullerene with amino acids. Scientific Reports, 2018, 8, 11400.	1.6	24
266	An Examination of the Electron Densities in a Series of Tripodal Cobalt Complexes Bridged by Magnesium, Calcium, Strontium, and Barium â€. Crystals, 2018, 8, 234.	1.0	0
267	Ligand Effect on Bonding in Gold(III) Carbonyl Complexes. Inorganic Chemistry, 2018, 57, 6161-6175.	1.9	21
268	Covalent character and electric field dependence of H2-AgX (X = F – I). Journal of Molecular Modeling, 2018, 24, 163.	0.8	1
269	Oxidative Coupling of Terminal Rhenium Pnictide Complexes. Angewandte Chemie, 2019, 131, 11082-11086.	1.6	13
270	Theoretical investigation on interactions of H2 absorption to CuXe cations I and II. European Physical Journal D, 2019, 73, 1.	0.6	0
271	A QTAIM and DFT study of the dizinc bond in non-symmetric [CpZn2Ln] complexes. Journal of Organometallic Chemistry, 2019, 898, 120878.	0.8	8
272	A combined experimental and theoretical analysis of the solid-state supramolecular self-assembly of N-(2,4-dichlorophenyl)-1-naphthamide: Synthesis, anticholinesterase potential and molecular docking analysis. Journal of Molecular Structure, 2019, 1197, 458-470.	1.8	15
273	pHâ€Responsive Switching Properties of a Waterâ€Soluble Metallamacrocyclic Phenylalaninehydroximate La(III)–Cu(II) Complex: Insight into Tuning Protonation Ligand States. European Journal of Inorganic Chemistry, 2019, 2019, 4328-4335.	1.0	8
274	A detailed computational investigation on the structural and spectroscopic properties of propolisbenzofuran B. Heliyon, 2019, 5, e02518.	1.4	14
275	Water-Soluble Chiral Y(III)–Cu(II) Metallamacrocyclic Phenylalaninehydroximate Complex. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2019, 45, 721-727.	0.3	7
276	Understanding the Stability Trend Along Light Lanthanide Complexes with an Ehtylenediamineâ€Type Ligand: A Quantum Chemical Study. ChemistrySelect, 2019, 4, 12368-12374.	0.7	8
277	<i>closo</i> -Carboranes as dual CHâ<¯i€ and BHâ<ī€ donors: theoretical study and biological significance. Physical Chemistry Chemical Physics, 2019, 21, 19944-19950.	1.3	13
278	Revisiting π backbonding: the influence of d orbitals on metal–CO bonds and ligand red shifts. Physical Chemistry Chemical Physics, 2019, 21, 20814-20821.	1.3	26
279	Quantifying individual (anti)bonding molecular orbitals' contributions to chemical bonding. Physical Chemistry Chemical Physics, 2019, 21, 20988-20998.	1.3	10
280	Cu(II) Complex of a Schiff Base Derived from Pyridoxal: Synthesis, Experimental Characterization, DFT Studies, and Aim Analysis. Journal of Structural Chemistry, 2019, 60, 1256-1266.	0.3	4
281	Computational analysis of M–O covalency in M(OC ₆ H ₅) ₄ (M = Ti,) Tj ET	QqQ 0 0 rg	gBT /Overloc

282	Dysprosium complexes bearing unsupported Dy ^{III} –Ge ^{II} /Sn ^{II} metal–metal bonds as single-ion magnets. Chemical Communications, 2019, 55, 8250-8253	2.2	20
	Communications, 2019, 33, 6230-6233.		

#	Article	IF	CITATIONS
283	Oxidative Coupling of Terminal Rhenium Pnictide Complexes. Angewandte Chemie - International Edition, 2019, 58, 10966-10970.	7.2	31
284	The first water-soluble polynuclear metallamacrocyclic Sr(<scp>ii</scp>)–Cu(<scp>ii</scp>) complex based on simple glycinehydroximate ligands. Dalton Transactions, 2019, 48, 10479-10487.	1.6	8
285	Polynuclear Glycinehydroximate Cu(II)–Gd(III) Metallamacrocyclic Complexes: Halochromic Properties. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2019, 45, 356-360.	0.3	5
286	DFT studies of the electron density distribution and donor-acceptor interactions in water-soluble aminohydroximate metallamacrocyclic Call and YIII complexes. Russian Chemical Bulletin, 2019, 68, 743-750.	0.4	10
287	How important is the coordinating atom in controlling magnetic anisotropy in uranium(<scp>iii</scp>) single-ion magnets? A theoretical perspective. Dalton Transactions, 2019, 48, 8976-8988.	1.6	20
288	Removing phenol contaminants from wastewater using graphene nanobuds: DFT and reactive MD simulation investigations. Journal of Molecular Liquids, 2019, 286, 110872.	2.3	11
289	Local Energy Dissipation/Transition in Field Effect Molecular Nanoelectronic Systems: a Quantum Mechanical Methodology. Communications in Theoretical Physics, 2019, 71, 441.	1.1	5
290	Activation of C–H, N–H, and O–H Bonds via Proton-Coupled Electron Transfer to a Mn(III) Complex of Redox-Noninnocent Octaazacyclotetradecadiene, a Catenated-Nitrogen Macrocyclic Ligand. Journal of the American Chemical Society, 2019, 141, 5699-5709.	6.6	11
291	Rydberg state mediated multiphoton ionization of (i- ⁷ -C ₇ H ₇)(i- ⁵ -C ₅ H ₅)Cr: DFT-supported experimental insights into the molecular and electronic structures of excited sandwich complexes. Physical Chemistry Chemical Physics, 2019, 21, 9665-9671.	1.3	2
292	Generation and Tunable Cyclization of Formamidinate Ligands in Carbonyl Complexes of Mn(I): An Experimental and Theoretical Study. Organometallics, 2019, 38, 916-925.	1.1	10
293	Theoretical Investigation on H2O2-Ng (He, Ne, Ar, Kr, Xe, and Rn) Complexes Suitable for Stereodynamics: Interactions and Thermal Chiral Rate Consequences. Frontiers in Chemistry, 2019, 6, 671.	1.8	5
294	Impact of confinement in multimolecular inclusion compounds of melamine and cyanuric acid. Physical Chemistry Chemical Physics, 2019, 21, 8205-8214.	1.3	5
295	Jahn-Teller effect in high spin d4 and d9 octahedral metal-complexes. Inorganica Chimica Acta, 2019, 486, 193-199.	1.2	30
296	Origin of the Photoinduced Geometrical Change of Copper(I) Complexes from the Quantum Chemical Topology View. Chemistry - A European Journal, 2019, 25, 775-784.	1.7	10
297	Theoretical Insights into Olefin Polymerization Catalyzed by Cationic Organo Rare-Earth Metal Complexes. , 2019, , 327-356.		10
298	A theoretical study of the bonding capabilities of the zincâ€zinc double bond. International Journal of Quantum Chemistry, 2019, 119, e25823.	1.0	5
299	Latin American contributions to quantum chemical topology. International Journal of Quantum Chemistry, 2019, 119, e25789.	1.0	6
300	X-ray diffraction and QTAIM calculations of the non-covalent intermolecular fluorine-fluorine interactions in tris(trifluoroacetylacetonato)-manganese(III). Journal of Molecular Structure, 2020, 1201, 127119.	1.8	6

Topological Analysis of the Electron Density in the Carbonyl Complexes M(CO) (M = Ca,) Tj ETQq0 0 0 rgBT /Overlock 10 1.1 21

304	Endohedral isomerism in model achiral and chiral La@C58N2 systems. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 231, 117791.	2.0	5
305	A Small Cationic Organo–Copper Cluster as Thermally Robust Highly Photo- and Electroluminescent Material. Journal of the American Chemical Society, 2020, 142, 373-381.	6.6	77
306	Conformational preference of nitroformazans: A computational study. Journal of Molecular Structure, 2020, 1203, 127463.	1.8	1
307	DFT performance in the IQA energy partition of small water clusters. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	2
308	Photochemical and antibacterial properties of ruthenium complex of N,N'-bis(benzimidazole-2yl-ethyl)ethylenediamine under visible light: Experimental and theoretical studies. Journal of Molecular Structure, 2020, 1203, 127377.	1.8	8
309	The adsorption of chlorofluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. Molecular Simulation, 2020, 46, 1405-1416.	0.9	33
310	The adsorption of chlorofluoromethane on pristine, and Al- and Ga-doped boron nitride nanosheets: a DFT, NBO, and QTAIM study. Journal of Molecular Modeling, 2020, 26, 287.	0.8	35
311	Low-coordinate Sm(<scp>ii</scp>) and Yb(<scp>ii</scp>) complexes derived from sterically-hindered 1,2-bis(imino)acenaphthene (Ar ^{BIG} -bian). Dalton Transactions, 2020, 49, 14445-14451.	1.6	12
312	Theoretical study of closo-borate derivatives of general type [BnHn-1COR]2– (nÂ=Â6, 10, 12; RÂ=ÂH, CH3,) Tj	ЕТ <u>О</u> 11	0.784314 r 15
313	Topological Analysis of Hydroxyquinoline Derivatives Interacting with Aluminum Cations or with an Al(111) Surface. Inorganic Chemistry, 2020, 59, 17916-17928.	1.9	2
314	From the Linnett–Gillespie model to the polarization of the spin valence shells of metals in complexes. Physical Chemistry Chemical Physics, 2020, 22, 24201-24212.	1.3	4
315	Theoretical investigation on interactions between coinage-metal and IIIA-atom. Journal of Molecular Modeling, 2020, 26, 227.	0.8	1
316	Treatment of adsorption of dioxane by using SiCNT toward efficient remediation of refractory organic contaminants from wastewater: DFT and DFTB-MD simulations. Journal of Molecular Liquids, 2020, 316, 113869.	2.3	4
317	Comparison of Chemical and Interpretative Methods: the Carbon–Boron Ï€â€Bond as a Test Case**. Chemistry - A European Journal, 2020, 26, 17230-17241.	1.7	2
318	On single-electron magnesium bonding formation and the effect of methyl substitution. RSC Advances, 2020, 10, 34413-34420.	1.7	1

#	Article	IF	CITATIONS
319	Block deformation analysis: Density matrix blocks as intramolecular deformation density. Journal of Computational Chemistry, 2020, 41, 2446-2458.	1.5	2
320	Theoretical study of the adsorption of amantadine on pristine, Al-, Ca-, P-, and As-doped boron nitride nanosheets: a PBC-DFT, NBO, and QTAIM study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	18
321	Partitioning a Molecule into the Atomic Basins and the Resultant Atomic Charges from Quantum Chemical Topology Analysis of the Kohn–Sham Potential. Journal of Physical Chemistry A, 2020, 124, 5023-5032.	1.1	3
322	Avoided spin coupling: an unexpected Ïf–Ïf diradical in global planar pentacoordinate carbon. Chemical Communications, 2020, 56, 7285-7288.	2.2	15
323	Hydrogen sulphide <scp>H₂S</scp> and noble gases (Ng = He, Ne, Ar, Kr, Xe, Rn) complexes: A theoretical study of their dynamics, spectroscopy, and interactions. International Journal of Quantum Chemistry, 2020, 120, e26266.	1.0	4
324	Chemical Bonding: The Journey from Miniature Hooks to Density Functional Theory. Molecules, 2020, 25, 2623.	1.7	11
325	Towards a Philosophy of Chemical Reactivity Through the Molecule in Atoms-of Concept. Axiomathes, 2020, , 1.	0.3	0
326	How to Stabilize a Heptagon-Containing C ₈₀ Cage by Endohedral Derivation. Inorganic Chemistry, 2020, 59, 8099-8107.	1.9	2
327	Metathesis of norbornene-derivatives bearing trimethylsilyl groups using Ru-alkylidene catalysts: An experimental and computational study. Journal of Organometallic Chemistry, 2020, 913, 121206.	0.8	4
328	Heteroleptic Nill complexes: Synthesis, structural characterization, computational studies and amoebicidal activity evaluation. Journal of Inorganic Biochemistry, 2020, 206, 111043.	1.5	3
329	Halogen⋯halogen interactions in decahalo-‹i>closo-carboranes: CSD analysis and theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 6122-6130.	1.3	12
330	How to Bend a Cumulene. Chemistry - A European Journal, 2020, 26, 4633-4639.	1.7	6
331	A sixteen-valence-electron carbon-group 13 family with global penta-atomic planar tetracoordinate carbon: an ionic strategy. Physical Chemistry Chemical Physics, 2020, 22, 3975-3982.	1.3	12
332	Theoretical study of adsorption of ethanol and acetone molecules by perfect and defected h-BN nanosheet. Superlattices and Microstructures, 2020, 139, 106403.	1.4	2
333	Taking a snapshot of the triplet excited state of an OLED organometallic luminophore using X-rays. Nature Communications, 2020, 11, 2131.	5.8	24
334	Structural, Spectroscopic, and Chemical Bonding Analysis of Zn(II) Complex [Zn(sal)](H2O): Combined Experimental and Theoretical (NBO, QTAIM, and ELF) Investigation. Crystals, 2020, 10, 259.	1.0	13
335	Anionâ‹â‹â‹Anion Attraction in Complexes of MCl ₃ ^{â^'} (M=Zn, Cd, Hg) with CN ^{â^'} . ChemPhysChem, 2020, 21, 1119-1125.	1.0	31
336	The adsorption of bromochlorodifluoromethane on pristine and Ge-doped silicon carbide nanotube: a PBC-DFT, NBO, and QTAIM study. Structural Chemistry, 2021, 32, 481-494.	1.0	27

#	Article	IF	CITATIONS
337	An Ultimate Investigation on the Adsorption of Amantadine on Pristine and Decorated Fullerenes C59X (X=Si, Ge, B, Al, Ga, N, P, and As): A DFT, NBO, and QTAIM Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 23-39.	1.0	28
338	Stereoisomeric Control in [RuCl 2 (PTA) 2 (2L)] Complexes (2L=2py or bpy): From Theoretical Calculations to a 2+2 Metallacycle of Pyridylporphyrins. European Journal of Inorganic Chemistry, 2021, 2021, 321-334.	1.0	0
339	Understanding structural and molecular properties of complexes of nucleobases and Au13 golden nanocluster by DFT calculations and DFT-MD simulation. Scientific Reports, 2021, 11, 435.	1.6	19
340	Laser spectroscopic and computational insights into unexpected structural behaviours of sandwich complexes upon ionization. Dalton Transactions, 2021, 50, 10729-10736.	1.6	5
341	Nanocrystalline Spinel Manganese Ferrite MnFe2O4: Synthesis, Electronic Structure, and Evaluation of Their Magnetic Hyperthermia Applications. Engineering Materials, 2021, , 335-348.	0.3	0
342	Theoretical assessments on the interaction between amino acids and the g-Mg ₃ N ₂ monolayer: dispersion corrected DFT and DFT-MD simulations. Physical Chemistry Chemical Physics, 2021, 23, 17440-17452.	1.3	43
343	Reversible Addition of Carbon Dioxide to Main Group Metal Complexes at Temperatures about 0 °C. Chemistry - A European Journal, 2021, 27, 5745-5753.	1.7	22
344	Metal–CO Bonding in Mononuclear Transition Metal Carbonyl Complexes. Jacs Au, 2021, 1, 623-645.	3.6	57
345	Orbitalâ€Free Quantum Crystallographic View on Noncovalent Bonding: Insights into Hydrogen Bonds, Ï€â‹â‹î€ and Reverse Electron Lone Pairâ‹â‹î€ Interactions. Chemistry - A European Journal, 2021, 2	7, ¹ 7789-7	809.
346	Structural Diversity and Argentophilic Interactions in Small Phosphine Silver(I) Thiolate Clusters. European Journal of Inorganic Chemistry, 2021, 2021, 2702-2711.	1.0	9
347	A DFT study of Se-decorated B12N12 nanocluster as a possible drug delivery system for ciclopirox. Computational and Theoretical Chemistry, 2021, 1201, 113246.	1.1	28
348	Stabilizing P≡P: P22–, P2â‹â€", and P20 as bridging ligands. CheM, 2021, 7, 1952-1962.	5.8	16
349	Strong intramolecular hydrogen bonding in confined amino acids. Journal of Molecular Graphics and Modelling, 2021, 106, 107913.	1.3	2
350	Interatomic Repulsion and the Pauli Principle. Journal of Chemical Education, 2021, 98, 2912-2918.	1.1	1
351	Comprehensive investigations of interaction properties of polylactic Acid‒Attapulgite composite by reactive molecular dynamics simulations and dispersion corrected DFT calculations. Current Applied Physics, 2021, 28, 78-86.	1.1	3
352	Pnictogen effects on the electronic interactions in the Lewis pair complexes Ph3EB(C6F5)3 (EÂ=ÂP, As,) Tj ETQq1	1.0.7843	14 rgBT /C
353	Frustrated Lewis Pairs based on Carbon···Carbon+ tetrel bonds: A DFT study. MarÃa de las Nieves Piña[a], Antonio Frontera[a], Tiddo. J. Mooibroek[b],* and Antonio Bauzá*[a]. ChemPhysChem, 2021, 22, 2478-2483.	1.0	3
354	Synthesis, structure, and PDE inhibiting activity of the anionic DNIC with 5-(3-pyridyl)-4H-1,2,4-triazole-3-thiolyl, the nitric oxide donor. Inorganica Chimica Acta, 2021, 527, 120559.	1.2	7

#	Article	IF	CITATIONS
355	Adsorption of acetone onto the pristine and Al-doped ZnO nanotubes: A dispersion corrected DFT study. Materials Science in Semiconductor Processing, 2021, 136, 106141.	1.9	3
356	Crystallographic and theoretical study of the atypical distorted octahedral geometry of the metal chromophore of zinc(II) bis((1R,2R)-1,2-diaminocyclohexane) dinitrate. Journal of Molecular Structure, 2022, 1248, 131488.	1.8	5
357	Selenium chalcogen bonds are involved in protein–carbohydrate recognition: a combined PDB and theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 17656-17662.	1.3	14
358	Perfluorinated Dialkoxysilanediols Resisting Selfâ€Condensation. European Journal of Inorganic Chemistry, 2021, 2021, 4402.	1.0	4
359	Ïf-Aromaticity Planar Pentacoordinate Beryllium Atoms. Inorganic Chemistry, 2021, 60, 16053-16058.	1.9	16
360	Ground electronic state description of thiourea coordination in homoleptic Zn ²⁺ , Ni ²⁺ and Co ²⁺ complexes using sulfur <i>K</i> -edge X-ray absorption spectroscopy. Journal of Synchrotron Radiation, 2021, 28, 1825-1838.	1.0	0
361	Effect of spectator ligands on haptotropic rearrangements of metalâ€azulene complexes European Journal of Inorganic Chemistry, 0, , .	1.0	0
362	Structures and Stability of Fullerenes, Metallofullerenes, and Their Derivatives. , 2016, , 1-66.		1
363	B-F bonding and reactivity analysis of mono- and perfluoro-substituted derivatives of closo-borate anions (6, 10, 12): A computational study. Polyhedron, 2022, 211, 115559.	1.0	8
364	Planar hexacoordinate gallium. Chemical Science, 2021, 12, 15067-15076.	3.7	15
365	An Ultimate Investigation on the Adsorption of Amantadine on Pristine and Decorated Fullerenes C ₅₉ X (X=Si, Ge, B, Al, Ga, N, P, and As): A DFT, NBO, and QTAIM Study. Journal of Theoretical and Computational Chemistry, 0, , .	1.8	1
366	Dispersion‒corrected DFT investigations on the interaction of glycine amino acid with metal organic framework MOF‒5. Physica B: Condensed Matter, 2022, 626, 413446.	1.3	36
367	Theoretical treatment of interaction of pyrazinamide with graphene and h-SiC monolayer: A DFT-D3 study. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 138, 115077.	1.3	13
368	Computational approach in lignin structural models: Influence of non-covalent intramolecular interactions on βO4 bond properties. Journal of Molecular Structure, 2022, 1251, 131938.	1.8	5
369	Structural and molecular properties of complexes of biomolecules and metal–organic frameworks: dispersion-corrected DFT treatment. Journal of Molecular Modeling, 2022, 28, 32.	0.8	3
370	Bond Dissociation Energies Reveal the Participation of d Electrons in f-Element Halide Bonding. Journal of Physical Chemistry A, 2022, 126, 272-285.	1.1	5
371	Molecular simulation of adsorption properties of thiol-functionalized titanium dioxide (TiO2) nanostructure for heavy metal ions removal from aqueous solution. Journal of Molecular Liquids, 2022, 346, 118281.	2.3	10
372	Steric paths in confined hydrogen molecule inside carbon nanorings and fullerenes. Computational and Theoretical Chemistry, 2022, 1209, 113590.	1.1	0

#	Article	IF	CITATIONS
373	Substituent Effects in Ï€â€Hole Regium Bonding Interactions Between Au(<i>p</i> â€Xâ€Py) ₂ Complexes and Lewis Bases: An <i>ab initio</i> Study. ChemPhysChem, 2022, , .	1.0	6
374	Molecular insights into the encapsulation of fluorouracil molecule inside the single-walled carbon nanotubes. Diamond and Related Materials, 2022, 124, 108900.	1.8	2
375	Sensing behaviour of monocyclic C18 and B9N9 analogues toward chemical warfare agents (CWAs); quantum chemical approach. Surfaces and Interfaces, 2022, 30, 101912.	1.5	13
376	Theoretical unraveling of the separation of trivalent Am and Eu ions by phosphine oxide ligands with different central heterocyclic moieties. Dalton Transactions, 2022, 51, 7118-7126.	1.6	10
377	Highly flexible phosphabenzenes: a missing coordination mode of 2,4,6-triaryl-λ ³ -phosphinines. Chemical Communications, 2022, 58, 6184-6187.	2.2	2
378	Protonation of Borylated Carboxonium Derivative [2,6-B10H8O2CCH3]â^': Theoretical and Experimental Investigation. International Journal of Molecular Sciences, 2022, 23, 4190.	1.8	8
381	Anionâ<ānion interaction within Ch(CH ₃)X ₄ ^{â^'} (Ch = S, Se, Te; X = Cl,) Tj E	то _д о о о 1.9	rgBT /Overlo
382	Molecular simulation investigations on the coating of Al-alloy surface by nano-SiO2-epoxy composite. Current Applied Physics, 2022, 39, 263-271.	1.1	1
383	Theoretical insights into the nature of the bonding between carbon monoxide and iron(II) phthalocyanine: How do QTAIM descriptors change as a function of the Fe–CO distance?. Chemical Physics Letters, 2022, 804, 139901.	1.2	1
384	Interaction of CO2 with TiO2/reduced graphene oxide as superior catalysts: Dispersion-corrected density functional theory simulation. Diamond and Related Materials, 2022, 128, 109279.	1.8	1

385	Metal-fullerene assisted adsorption of dichlorosilane: DFT assessments. Computational and Theoretical Chemistry, 2022, 1216, 113868.	1.1	1
386	Water-Soluble 15-Metallacrown-5 Complexes: Molecular Structures and Properties. , 2022, , 277-315.		1
387	Interaction-determined extraction capacity between rare earth ions and extractants: taking lanthanum and lutetium as models through theoretical calculations. Inorganic Chemistry Frontiers, 2022, 9, 5360-5370.	3.0	4
388	The <i>N</i> , <i>N</i> , <i>N</i> -trimethylammonium moiety as tetrel bond donor site: crystallographic and computational studies. Physical Chemistry Chemical Physics, 2022, 24, 24892-24901.	1.3	2
389	A two-dimensional Be ₂ Au monolayer with planar hexacoordinate s-block metal atoms: a superconducting global minimum Dirac material with two perfect Dirac node-loops. Chemical Science, 2022, 13, 11099-11109.	3.7	5
390	Ionization of Decamethylmanganocene: Insights from the DFT-Assisted Laser Spectroscopy. Molecules, 2022, 27, 6226.	1.7	2
391	Theoretical Insight into B–C Chemical Bonding in Closo-Borate [BnHnâ^'1CH3]2â^' (n = 6, 10, 12) and Monocarborane [CBnHnCH3]â^' (n = 5, 9, 11) Anions. Inorganics, 2022, 10, 186.	1.2	2
392	A coumarin based Schiff Base: An effective colorimetric sensor for selective detection of F– ion in real samples and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 286, 121964.	2.0	10

		CITATION REF	PORT	
#	Article		IF	CITATIONS
393	The amphoteric role of nitrogen in the NX ₂ unit within crystals. CrystEngComm, 0, , .		1.3	0
394	Uncovering the role of non-covalent interactions in solid-state photoswitches by non-spherical structure refinements with NoSpherA2. Faraday Discussions, 0, 244, 370-390.		1.6	3
395	The reactivity of antimony and bismuth <i>N</i> , <i>C</i> , <i>N</i> -pincer compounds toward K[BEt ₃ H] – the formation of heterocyclic compounds <i>vs</i> . element–element bonds <i>vs.</i> stable terminal Sb–H bonds. Dalton Transactions, 2022, 52, 218-227.		1.6	1
396	DFT investigation of a Zn-doped carbon nanocone for the drug delivery of methylated aspirins. Computational and Theoretical Chemistry, 2023, 1220, 113976.		1.1	3
397	Non-covalent interactions towards 2-(4-(2,2-dicyanovinyl) benzylidene)malononitrile packing polymorphism due to solvent effect. Experimental and theoretical spectroscopy approach. Journal c Molecular Structure, 2023, 1275, 134674.	ſ	1.8	1
398	Molecular simulation investigations on interaction properties of the teriflunomide–chitosan complex in aqueous solution. Journal of Physics and Chemistry of Solids, 2023, 174, 111171.		1.9	19
399	Adsorption behavior of methylene blue on graphene and hexagonal boron nitride monolayers in aqueous solution: A first-principles treatment. Journal of Physics and Chemistry of Solids, 2023, 174 111151.	ŀ,	1.9	2
400	Theoretical Analysis of Polynuclear Zinc Complexes Isolobally Related to Hydrocarbons. International Journal of Molecular Sciences, 2022, 23, 14858.		1.8	1
401	Detection of hydrogen fluoride (HF) gas by Mg12O11-X (X = S, P, N, and B) nanosurfaces. Chemica Physics Impact, 2022, 5, 100129.		1.7	20
402	Energy property and covalency of H ₂ S···X (X = N ₂ , CO, CS and SiO) h bond. Physica Scripta, 2023, 98, 015407.	ydrogen	1.2	0
403	Hydroboration of a Diolate Complex Obtained by Carbon Dioxide Capture with Acenaphthenediimir Aluminum Hydride. Organometallics, 2023, 42, 123-131.	ie	1.1	6
404	xmins:mml="http://www.w3.org/1998/Math/Math/MathML"altimg="si1.svg" display="inline" id="d1e1928"> <mml:msup><mml:mrow /><mml:mrow><mml:mo>I<mml:mo>)</mml:mo>xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si2.svg" display="inline"</mml:mo></mml:mrow></mml:mrow </mml:msup>	nml:mrow> <td>າຫຼາອກrov</td> <td>v>≰/mml:msi</td>	າ ຫຼາ ອກrov	v> ≰ /mml:msi
405	Id="d1e1211" summarized summarized with mercaptopurine anti-cancer drug. Physica B: Condensed Matter, 2023, , 414547.		1.3	0
406	PALLADIUM(II) COMPLEX WITH TETRAHYDROBENZOXAZINOBENZOXOSINE: SYNTHESIS, ELECTRO MOLECULAR STRUCTURES. Journal of Structural Chemistry, 2022, 63, 1963-1972.	NIC AND	0.3	0
407	Introduction to QTAIM and beyond. , 2023, , 1-19.			0
408	Applications of the quantum theory of atoms in molecules and the interacting quantum atoms methods to the study of hydrogen bonds. , 2023, , 431-468.			1
409	Spin polarization of the atomic valence shell in metal complexes. , 2023, , 389-406.			0
410	Assessing the drug delivery of ibuprofen by the assistance of metal-doped graphenes: Insights from density functional theory. Diamond and Related Materials, 2023, 135, 109.893.		1.8	19

#	Article	IF	CITATIONS
411	Adsorption of thiotepa anticancer by the assistance of aluminum nitride nanocage scaffolds: A computational perspective on drug delivery applications. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2023, 666, 131276.	2.3	0
412	Computational investigations on the 4–cyanopyridine adsorbed on ZnO–graphene oxide nanocomposite toward the efficient performance of surface–enhanced Raman scattering. Diamond and Related Materials, 2023, 133, 109693.	1.8	0
413	Experimental and theoretical studies on the extraction behavior of Cf(<scp>iii</scp>) by NTAamide(C8) ligand and the separation of Cf(<scp>iii</scp>)/Cm(<scp>iii</scp>). RSC Advances, 2023, 13, 3781-3791.	1.7	2
414	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5]â^: Theoretical and Experimental Study. Molecules, 2023, 28, 1757.	1.7	1
415	Therapeutic Potential of B ₁₂ N ₁₂ -X (X = Au, Os, and Pt) Nanostructured as Effective Fluorouracil (5Fu) Drug Delivery Materials. ACS Applied Bio Materials, 2023, 6, 1146-1160.	2.3	23
416	NAl4X4+ (X = S, Se, Te): Clusters with a planar tetracoordinate nitrogen and significantly improved stability. Journal of Chemical Physics, 2023, 158, .	1.2	2
420	Titanium(II) as a Fuel Atom in Energetic Materials. Inorganic Chemistry, 2023, 62, 9285-9290.	1.9	0