

# Characterization of C-H-O Hydrogen Bonds on the Basis of

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Citation Report

#	ARTICLE	IF	CITATIONS
4	The C-H...O Hydrogen Bond: Structural Implications and Supramolecular Design. <i>Accounts of Chemical Research</i> , 1996, 29, 441-449.	7.6	1,802
5	Hydration of C-H groups in tRNA. <i>Faraday Discussions</i> , 1996, 103, 151-173.	1.6	47
6	Theoretical study of intramolecular hydrogen bonding and molecular geometry of 2-trifluoromethylphenol. <i>Journal of Computational Chemistry</i> , 1996, 17, 1804-1819.	1.5	24
7	MORPHY, a program for an automated atoms in molecules analysis. <i>Computer Physics Communications</i> , 1996, 93, 212-240.	3.0	239
8	Infrared Matrix Isolation Study of Acetone and Methanol in Solid Argon. <i>The Journal of Physical Chemistry</i> , 1996, 100, 17124-17132.	2.9	72
9	C-H...C Hydrogen bonding involving ylides. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, 2241-2248.	0.9	28
10	A Charge Density Analysis of Cationic and Anionic Hydrogen Bonds in a Proton Sponge Complex. <i>Journal of the American Chemical Society</i> , 1997, 119, 11502-11509.	6.6	103
11	Topological analysis of hydrogen bonding interactions involving C-H...O bonds. <i>Computational and Theoretical Chemistry</i> , 1997, 401, 77-85.	1.5	39
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18	A method to integrate an atom in a molecule without explicit representation of the interatomic surface. <i>Computer Physics Communications</i> , 1998, 108, 180-190.	3.0	101
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1244	Intramolecular photoinduced proton transfer in 2-(2-hydroxyphenyl)benzazole family: A TD-DFT quantum chemical study. <i>Chemical Physics</i> , 2014, 444, 66-76.	0.9	22
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1276	Physical Nature of Interactions in Zn <sup>II</sup> Complexes with 2,2'-Bipyridyl: Quantum Theory of Atoms in Molecules (QTAIM), Interacting Quantum Atoms (IQA), Noncovalent Interactions (NCI), and Extended Transition State Coupled with Natural Orbitals for Chemical Valence (ETS-NOCV) Comparative Studies. <i>Journal of Physical Chemistry A</i> , 2014, 118, 623-637.	1.1	81
1277	The conformational behavior, geometry and energy parameters of Menshutkin-like reaction of O-isopropylidene-protected glycofuranoid mesylates in view of DFT calculations. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 52, 91-102.	1.3	4
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1313	Substituent effects on cooperativity between lithium bonds. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 295-301.	1.0	16
1314	Cooperativity effects between $\pi$ -hole interactions: a theoretical evidence for mutual influence between chalcogen bond and halogen bond interactions in $F_2S_2\text{-}NXCX\text{-}NCY$ complexes ( $X = Tl, Pb, Bi, Po, At, Rn$ )	1.1	14

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1331	Anticancer drug IUdR and other 5-halogen derivatives of 2"deoxyuridine: conformers, hydrates, and structure"activity relationships. <i>Structural Chemistry</i> , 2014, 25, 53-69.	1.0	10
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1338	Can 2 $\alpha$ -acylpyrroles form an intramolecular hydrogen bond?. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 652-662.	0.9	3
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1342	The dual role of halogen, chalcogen, and pnictogen atoms as Lewis acid and base: Triangular XBr:SHX:PH <sub>2</sub> X complexes (X = F, Cl, Br, CN, NC, OH, NH <sub>2</sub> ), and OCH <sub>3</sub> Tj ETQ 0 0 0 0	0.0	0
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1356	Mutual influence between anionâ€“ $\text{F}^-$ and pnictogen bond interactions: The enhancement of $\text{P}\delta^- \text{N}$ and $\text{P}\delta^- \text{O}$ interactions by an anionâ€“ $\text{F}^-$ bond. Journal of Molecular Graphics and Modelling, 2015, 57, 99-105.	1.3	22
1357	Negative hyperconjugation and red-, blue- or zero-shift in $\text{X}\delta^+ \text{Z}\delta^- \text{Y}$ complexes. Faraday Discussions, 2015, 177, 33-50.	1.6	20
1358	Acidâ€“Base Formalism in Dispersion-Stabilized $\text{S}\delta^+ \text{H}\delta^- \text{A}\delta^- \text{Y}$ ( $\text{Y} = \text{O}, \text{S}$ ) Hydrogen-Bonding Interactions. Journal of Physical Chemistry A, 2015, 119, 1117-1126.	1.1	25
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1372	Theoretical study on cooperative interplay between anion-π and chalcogen-bonding interactions. <i>Molecular Physics</i> , 2015, 113, 1442-1450.	0.8	14
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1386	What is Common for Dihydrogen Bond and σ-hole Interaction? Theoretical Analysis and Experimental Evidences. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 159-187.	0.6	3
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1408	Is There Any Preferential Interaction of Ions of Ionic Liquids with DMSO and H <sub>2</sub> O? A Comparative Study from MD Simulation. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6686-6695.	1.2	39
1409	Hydrogen Bonds Involving Sulfur: New Insights from ab Initio Calculations and Gas Phase Laser Spectroscopy. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , 15-45.	0.6	40
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1413	Meta-Hybrid Density Functional Theory Study of Adsorption of Imidazolium- and Ammonium-Based Ionic Liquids on Graphene Sheet. <i>Journal of Physical Chemistry C</i> , 2015, 119, 7095-7108.	1.5	68
1414	A computational study of intramolecular hydrogen bonds breaking/formation: impact on the structural flexibility of the ranitidine molecule. <i>Journal of Molecular Modeling</i> , 2015, 21, 94.	0.8	1
1415	Noncovalent Forces. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2015, , .	0.6	116
1416	Vibrational studies (FTIR and Raman), conformational analysis, NBO, HOMO-LUMO and reactivity descriptors of S-methyl thiobutanoate, CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(O)SCH <sub>3</sub> . <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 149, 408-418.	2.0	4
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1424	Tuning of chalcogen bonds by cation- $\pi$ interactions: cooperative and diminutive effects. <i>Journal of Molecular Modeling</i> , 2015, 21, 300.	0.8	8

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1427	QM study of complexation between natural bilirubin and poly-terthiophene carboxylic acidâ€“Mn(II) as a biosensor: Temperature and interferences effect. <i>Journal of Theoretical and Computational Chemistry</i> , 2015, 14, 1550048.	1.8	1
1428	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained C $\pm$ -Tetrasubstituted $\alpha$ -Amino Acids in Aib-based Peptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14003-14013.	1.2	18
1429	Interplay between hydrogen bond and single-electron tetrel bond: H <sub>3</sub> Câˆ“COX <sub>2</sub> âˆ“HY and H <sub>3</sub> Câˆ“CSX <sub>2</sub> âˆ“HY (X = F, Cl, Br, I). <i>Journal of Physical Chemistry A</i> , 2015, 119, 101-106.	1.1	19
1430	Intermolecular atomâ€“atom bonds in crystals â€“ a chemical perspective. <i>IUCr</i> , 2015, 2, 159-160.	1.0	63
1431	The conjugates of ferrocene-1,1â€“2-diamine and amino acids. A novel synthetic approach and conformational analysis. <i>Dalton Transactions</i> , 2015, 44, 16405-16420.	1.6	21
1432	Rotational spectroscopy of methyl benzoylformate and methyl mandelate: structure and internal dynamics of a model reactant and product of enantioselective reduction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21942-21949.	1.3	5
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1434	Theoretical study on the structure and cationâ€“anion interaction of triethylammonium chloroaluminate ionic liquid. <i>Computational and Theoretical Chemistry</i> , 2015, 1073, 67-74.	1.1	13
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1436	Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach. <i>New Journal of Chemistry</i> , 2015, 39, 9800-9812.	1.4	53
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1438	Abnormal synergistic effects between Lewis acidâ€“base interaction and halogen bond in F <sub>3</sub> Bâˆ“NCAâˆ“NCM. <i>Molecular Physics</i> , 2015, 113, 3809-3814.	0.8	23
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1441	Organic alloys of room temperature liquids thiophenol and selenophenol. <i>Chemical Communications</i> , 2015, 51, 14255-14258.	2.2	46
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1444	An ab initio study on tunability of $\pi$ -hole interactions in XHS:PH <sub>2</sub> Y and XH <sub>2</sub> P:SHY complexes (X = F, Cl, Br). <i>J. ETQ</i> , 2015, 1, 0.78-0.81.	0.8	20
1445	Exploring physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs). <i>Journal of Molecular Liquids</i> , 2015, 209, 14-24.	2.3	17
1446	The C O rotation in the gaseous glycine. An energy decomposition analysis study. <i>Chemical Physics Letters</i> , 2015, 640, 194-200.	1.2	4
1447	Probing molecular interactions underlying imidazolium and pyridinium based ionic liquids. <i>Journal of Molecular Liquids</i> , 2015, 212, 885-899.	2.3	11
1448	Theoretical studies of traditional and halogen-shared halogen bonds: the doped all-metal aromatic clusters MA <sub>3</sub> (M = Al, Si, Ge, Sn, Pb) as halogen bond acceptors. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	3
1449	Symmetry-Adapted Perturbation Theory study on interactions between small cycloalkanes. <i>Chemical Physics Letters</i> , 2015, 640, 147-152.	1.2	1
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1451	Mechanism of Stabilization of Helix Secondary Structure by Constrained C <sub>1</sub> -Tetrasubstituted $\alpha$ -Amino Acids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1350-1361.	1.2	25
1452	Assessment of hydrophobic interactions and their contributions through the analysis of the methane dimer. <i>Journal of Computational Chemistry</i> , 2015, 36, 361-375.	1.5	16
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1456	Investigating the nature of intermolecular and intramolecular bonds in noble gas containing molecules. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 165-171.	1.0	1
1457	A combined experimental and DFT study of a novel unsymmetrical azine 2-(4-methoxybenzylidene)-1-(1-(4-isobutylphenyl) ethylidene) hydrazine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 460-473.	2.0	11
1458	3-Chlorotyramine Acting as Ligand of the Dopamine Receptor. <i>Molecular Modeling, Synthesis and Receptor Affinity</i> . <i>Molecular Informatics</i> , 2015, 34, 28-43.	1.4	10
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1463	Organic light emitting diodes (OLED) based on helical structures containing 7-membered fused rings. <i>Dyes and Pigments</i> , 2015, 114, 184-195.	2.0	27
1464	The significant role of the intermolecular $CH \cdots O/N$ hydrogen bonds in governing the biologically important pairs of the DNA and RNA modified bases: a comprehensive theoretical investigation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 1624-1652.	2.0	80
1465	Molecular structure, vibrational spectra, AIM, HOMO-LUMO, NBO, UV, first order hyperpolarizability, analysis of 3-thiophenecarboxylic acid monomer and dimer by Hartree-Fock and density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1227-1242.	2.0	79
1466	A DFT approach to the charge transport related properties in columnar stacked $\pi$ -conjugated N-heterocycle cores including electron donor and acceptor units. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 605-618.	1.3	12
1467	Novel synthetic ester of Brassicasterol, DFT investigation including NBO, NLO response, reactivity descriptor and its intramolecular interactions analyzed by AIM theory. <i>Journal of Molecular Structure</i> , 2015, 1083, 72-81.	1.8	43
1468	Synthesis, conformational, spectroscopic and chemical reactivity analysis of 2-cyano-3-(1H-pyrrol-2-yl)acrylohydrazide using experimental and quantum chemical approaches. <i>Journal of Molecular Structure</i> , 2015, 1082, 118-130.	1.8	13
1469	Atomic energy analysis of cooperativity, anti-cooperativity, and non-cooperativity in small clusters of methanol, water, and formaldehyde. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 328-336.	1.1	23
1470	Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and) <i>Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 38</i> <i>Molecular Simulation</i> , 2015, 41, 633-652.	0.9	10
1471	Enhancement effect of lithium bonding on the strength of $\pi$ -hole interactions in $O_2 \cdots S \cdots NLi \cdots NCX$ and $O_2 \cdots S \cdots CNLi \cdots CNX$ complexes ( $X = H, F, CN, OH$ and) <i>Tj ETQq0 0 0 rgBT /C</i>	0.9	10
1472	Ab initio calculations of cooperativity effects on chalcogen bonding: linear clusters of $(OCS)_2 \cdots 8$ and $(OCS)_2 \cdots 8$ . <i>Structural Chemistry</i> , 2015, 26, 199-206.	1.0	35
1473	Molecular structure and vibrational spectroscopic studies on 2-furanacetic acid monomer and dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 579-593.	2.0	4
1474	On the properties of $S \cdots O$ and $S \cdots \pi$ noncovalent interactions: the analysis of geometry, interaction energy and electron density. <i>New Journal of Chemistry</i> , 2015, 39, 1611-1618.	1.4	36
1475	Molecular structure and conformations of caramboxin, a natural neurotoxin from the star fruit: A computational study. <i>Journal of Molecular Structure</i> , 2015, 1079, 274-280.	1.8	2
1476	Six questions on topology in theoretical chemistry. <i>Computational and Theoretical Chemistry</i> , 2015, 1053, 2-16.	1.1	99
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1478	Tetrel-Hydride Interaction between $XH_3 \cdots F$ ( $X = C, Si, Ge, Sn$ ) and $HM$ ( $M = Li, Na, BeH, MgH$ ). <i>Journal of Physical Chemistry A</i> , 2015, 119, 2217-2224.	1.1	79

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1480	The nature of interactions between [Cu <sub>2</sub> Cl <sub>3</sub> ] <sup>-</sup> -based ionic liquid and thiophene – A theoretical study. <i>Journal of Saudi Chemical Society</i> , 2016, 20, 303-306.	2.4	5
1481	Mononuclear gallium (III) complexes based on salicylaldehydes: Theoretical study of structures, topological and NBO analysis of hydrogen bonding interactions involving O-H...O bonds. <i>Arabian Journal of Chemistry</i> , 2016, 9, S361-S372.	2.3	5
1482	Is conformation a fundamental descriptor in QSAR? A case for halogenated anesthetics. <i>Beilstein Journal of Organic Chemistry</i> , 2016, 12, 760-768.	1.3	12
1483	Decomposition of Intermolecular Interactions in the Crystal Structure of Some Diacetyl Platinum(II) Complexes: Combined Hirshfeld, AIM, and NBO Analyses. <i>Molecules</i> , 2016, 21, 1669.	1.7	13
1484	Topological Analysis of Electron Density – Quantum Theory of Atoms in Molecules. , 2016, , 359-384.		5
1485	C <sub>2</sub> H <sub>5</sub> OH...HX (X=OH, SH, F) interactions: Is there a carbon bond?. <i>Journal of Chemical Sciences</i> , 2016, 128, 1191-1198.	0.7	1
1486	Structure and electrochemical properties for complexes of nitrocompounds with inorganic ions: A theoretical approach. <i>Journal of Computational Chemistry</i> , 2016, 37, 1206-1213.	1.5	2
1487	Combined spectroscopic and quantum chemical studies of ezetimibe. <i>Journal of Molecular Structure</i> , 2016, 1125, 193-203.	1.8	12
1488	Structural, electronic and QTAIM analysis of host-guest interaction of Warfarin with $\beta$ -cyclodextrin and calix[4]arene. <i>Journal of Molecular Liquids</i> , 2016, 221, 885-895.	2.3	15
1489	Fluoroethersols: The Key Role of Intramolecular Hydrogen Bonding in Conformational Preference and Hydrogen Bond Acidity. <i>ChemPhysChem</i> , 2016, 17, 2702-2709.	1.0	12
1490	Photoswitching in nanostructured benzofuro[3,2-b]pyridin-9-ol and benzothio[3,2-b]pyridin-9-ol compounds as red- and yellow-light-emitting molecules: A TD-DFT approach. <i>Dyes and Pigments</i> , 2016, 134, 106-117.	2.0	10
1491	Intramolecular Hydrogen Bonds in Low-Molecular-Weight Polyethylene Glycol. <i>ChemPhysChem</i> , 2016, 17, 1143-1153.	1.0	31
1492	Deciphering Noncovalent Interactions Accompanying 7,7,8,8-tetracyanoquinodimethane Encapsulation within Biphenylarenes: Nucleus-Independent Chemical Shifts Approach. <i>ChemPhysChem</i> , 2016, 17, 2197-2209.	1.0	27
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1496	Hydrogen bonding in alcohol-ethylene oxide and alcohol-ethylene sulfide complexes. <i>RSC Advances</i> , 2016, 6, 91233-91242.	1.7	20

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1498	Halides with Fifteen Aliphatic C-H...Anion Interaction Sites. <i>Scientific Reports</i> , 2016, 6, 30123.	1.6	7
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1501	Influence of the protonation of pyridine nitrogen on pnictogen bonding: competition and cooperativity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11348-11356.	1.3	16
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1504	Exploration of Binding Interactions of Cu <sup>2+</sup> with Penicillamine and its O- and Se- Analogues in Both Gas and Aqueous Phases: A Theoretical Approach. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3467-3478.	1.2	7
1505	The mutual influence of Y-H...N and H-H...H interactions in XHY-H-NCH-H-M complexes (X = F, Cl, Br; Y = S, Se; Z = O, S, Se). <i>Journal of Chemistry</i> , 2016, 94, 567-573.	0.6	3
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1508	A substituted sulfonamide and its Co (II), Cu (II), and Zn (II) complexes as potential antifungal agents. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 51-62.	2.5	43
1509	Structure of isothiocyanic acid dimers. Theoretical and FTIR matrix isolation studies. <i>Chemical Physics Letters</i> , 2016, 652, 46-49.	1.2	6
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1512	Molecular structure, hydrogen-bonding patterns and topological analysis (QTAIM and NCI) of 5-methoxy-2-nitroaniline and 5-methoxy-2-nitroaniline with 2-amino-5-nitropyridine (1:1) co-crystal. <i>Journal of Molecular Structure</i> , 2016, 1119, 505-516.	1.8	18
1513	The mutual influence between $\pi$ -hole pnictogen bonds and $\sigma$ -hole halogen bonds in complexes of PO <sub>2</sub> Cl and XCN/C <sub>6</sub> H <sub>6</sub> (X = F, Cl, Br). <i>Structural Chemistry</i> , 2016, 27, 1427-1437.	1.0	18
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1544	An analysis of the experimental and theoretical charge density distributions of the piroxicamâ€•saccharin co-crystal and its constituents. <i>RSC Advances</i> , 2016, 6, 81578-81590.	1.7	18
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1546	Experimental and theoretical study of intramolecular Oâ€•O interaction in structurally rigid Î²-keto carboxylic esters. <i>RSC Advances</i> , 2016, 6, 91689-91693.	1.7	14
1547	Hydrogen bonds in methaneâ€•water clusters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23508-23515.	1.3	16
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1564	Two rhodamine 6G derivative compounds: a structural and fluorescence single-crystal study. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 684-692.	0.5	9
1565	Br $\cdots$ Br and van der Waals interactions along a homologous series: crystal packing of 1,2-dibromo-4,5-dialkoxybenzenes. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 693-701.	0.5	2
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1567	Two- and Three-Centered Hydrogen Bonds Involving Organic Fluorine Stabilize Conformations of Hydrazide Halo Derivatives: NMR, IR, QTAIM, NCI, and Theoretical Evidence. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7810-7816.	1.1	13
1568	Hydrogen bonding in cyclic complexes of carboxylic acid-sulfuric acid and their atmospheric implications. <i>RSC Advances</i> , 2016, 6, 71733-71743.	1.7	26
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1572	Z-Isomers of (4 <sup>+</sup> 6 <sup>+</sup> , 2 <sup>+</sup> 1 <sup>+</sup> O <sup>+</sup> 1 <sup>+</sup> )-phenylflavan substituted with R <sup>2</sup> =R-OH. Conformational properties, electronic structure and aqueous solvent effects. <i>Journal of Molecular Modeling</i> , 2016, 22, 187.	0.8	3
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1581	The Crystal Structure and Behavior of Fenamic Acid-Acridine Complex Under High Pressure. <i>Journal of Pharmaceutical Sciences</i> , 2016, 105, 3487-3495.	1.6	3
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1583	Dielectric Relaxation Study at Ambient and Elevated Pressure of the Modeled Lipophilic Drug Fenofibrate. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11298-11306.	1.2	17
1584	Homonuclear chalcogen...chalcogen bond interactions in complexes pairing YO <sub>3</sub> and YHX molecules (Y=S, Se; X=H, Cl, Br, CCl <sub>4</sub> , NC, OH). <i>J. ETQ</i> 13	1.0	13
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1586	Highly stable naphthalene core based novel cleft-shaped strain molecule: influence of intermolecular H-bonding architectures. <i>RSC Advances</i> , 2016, 6, 59574-59581.	1.7	5
1587	Cooperativity of intermolecular hydrogen bonds in microsolvated DMSO and DMF clusters: a DFT, AIM, and NCI analysis. <i>Journal of Molecular Modeling</i> , 2016, 22, 151.	0.8	40
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1894	Hydrogen-bond network in liquid Formamide Methanol mixture as studied by neutron scattering and density functional theory. <i>Journal of Molecular Liquids</i> , 2018, 271, 8-15.	2.3	2

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1895	Theoretical and experimental approach to the investigation of hyperpolarizability and charge transfer characteristics of NLO active 2,3,4,5-pentamethoxy chalcone with silver atoms adsorbed. <i>Optical Materials</i> , 2018, 84, 409-421.	1.7	13
1896	Explicit Aqueous Solvation Treatment of Epinephrine from Car Parrinello Molecular Dynamics: Effect of Hydrogen Bonding on the Electronic Absorption Spectrum. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8439-8450.	1.2	7
1897	Autocatalytic Synthesis of Bifluoride Ionic Liquids by SuFEx Click Chemistry. <i>Angewandte Chemie</i> , 2018, 130, 16237-16241.	1.6	15
1898	Autocatalytic Synthesis of Bifluoride Ionic Liquids by SuFEx Click Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 16005-16009.	7.2	38
1899	Characterizing Hydrogen-Bond Interactions in Pyrazinetetracarboxamide Complexes: Insights from Experimental and Quantum Topological Analyses. <i>Inorganic Chemistry</i> , 2018, 57, 9775-9778.	1.9	3
1900	Fine-tuning the photophysical properties of the five quinolin based nanophotoswitches in the gas phase, polar and nonpolar solvents: A TD-DFT approach. <i>Journal of Luminescence</i> , 2018, 204, 230-243.	1.5	2
1901	Acidic and basic sites of M2DEBDC (M = Mg or Mn and E = O or S) acting as catalysts for cyanosilylation of aldehydes. <i>Polyhedron</i> , 2018, 154, 98-107.	1.0	7
1902	Theoretical modeling of argentophilic interactions in [Ag(CN) <sub>2</sub> ] <sub>3</sub> trimer found in a copper(II) complex of cis-1,2-diaminocyclohexane (Dach), [Cu(Dach) <sub>2</sub> -Ag(CN) <sub>2</sub> -Cu(Dach) <sub>2</sub> ][Ag(CN) <sub>2</sub> ] <sub>3</sub> . <i>Chemical Physics Letters</i> , 2018, 709, 11-15.	1.2	4
1903	An experimental and theoretical study on the kinetics of the reaction between 4-hydroxycyclohexanone CH <sub>3</sub> CH <sub>2</sub> C(O)CH(OH)CH <sub>2</sub> CH <sub>2</sub> and OH radicals. <i>International Journal of Chemical Kinetics</i> , 2018, 50, 556-567.	1.0	5
1904	Solution equilibria of aromatic dinitroso compounds: a combined NMR and DFT study. <i>Structural Chemistry</i> , 2018, 29, 1489-1497.	1.0	8
1905	Clustering mechanism of oxocarboxylic acids involving hydration reaction: Implications for the atmospheric models. <i>Journal of Chemical Physics</i> , 2018, 148, 214303.	1.2	22
1906	Effect of charge transfer with spectral analysis on the antibacterial compound 4-(Dimethyl amino) pyridine: 3,5-Dinitrobenzoic acid: Experimental and theoretical perspective. <i>Journal of Molecular Structure</i> , 2018, 1171, 511-526.	1.8	16
1907	Deconvolution of conformational equilibria in methimazolium-based ionic liquid ion pair: Infrared spectroscopic and computational study. <i>Journal of Molecular Liquids</i> , 2018, 266, 194-202.	2.3	1
1908	Influence of Cation Size on the Structural Features and Interactions in Tertiary Alkylammonium Trifluoroacetates: A Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5878-5885.	1.1	15
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1910	Do amino acids prefer only certain backbone structures? Steering through the conformational maze of l-threonine using matrix isolation infrared spectroscopy and ab initio studies. <i>Journal of Molecular Structure</i> , 2019, 1175, 117-129.	1.8	6
1911	Combined spectroscopic and quantum chemical approach to study the effect of hydrogen bonding interactions in ezetimibe. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 206, 246-253.	2.0	9
1912	Theoretical insights into the hydrogen bonding interaction in the complexation of epinephrine with uracil. <i>Journal of Molecular Modeling</i> , 2019, 25, 252.	0.8	10

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1914	Electronic structure and spectral characteristics of alkyl substituted imidazolium based dication-X <sub>2</sub> (X=Br, BF <sub>4</sub> , PF <sub>6</sub> and CF <sub>3</sub> SO <sub>3</sub> ) complexes from theory. <i>Journal of Molecular Liquids</i> , 2019, 293, 111548.	2.3	5
1915	DFT investigation of role of Nâ€“Hâ€“O and Nâ€“Hâ€“I interactions in the stabilization of the hydrogen bonded complexes of anisole with aromatic amines. <i>Heliyon</i> , 2019, 5, e02155.	1.4	15
1916	Synthesis, characterization, DFT calculations, electric and dielectric properties of (C <sub>6</sub> H <sub>10</sub> (NH <sub>3</sub> ) <sub>2</sub> ) CdCl <sub>4</sub> H <sub>2</sub> O organic-inorganic hybrid compound. <i>Journal of Molecular Structure</i> , 2019, 1198, 126887.	1.8	7
1917	Host-guest interactions accompanying the cationic nitrogen heterocyclic guests encapsulation within pillar[5]arene: A theoretical research. <i>Journal of Molecular Structure</i> , 2019, 1198, 126862.	1.8	8
1918	Triel bonds in RZ <sub>2</sub> ÂˆÂˆNH <sub>3</sub> : hybridization, solvation, and substitution. <i>Journal of Molecular Modeling</i> , 2019, 25, 219.	0.8	8
1919	Electronic substituent effect on Se-Hâ€“N hydrogen bond: A computational study of para-substituted pyridine-SeH <sub>2</sub> complexes. <i>Chemical Physics Letters: X</i> , 2019, 737, 100031.	2.1	9
1920	Lack of resonance assistance in a classical intramolecular hydrogen bond: An exploration from quantum theory of atomsâ€“molecules perspective. <i>Journal of Physical Organic Chemistry</i> , 2019, 32, e3999.	0.9	5
1921	A quantitative study of weak noncovalent interactions in two pyridine isomers containing nitrile and thiophene moieties: a combined X-ray and theoretical investigation. <i>Journal of Chemical Sciences</i> , 2019, 131, 1.	0.7	7
1922	Effects of Electronic Structure of Adjacent Carbon on the Strength of Câ€“Fâ€“Hâ€“F Organofluorine Hydrogen Bonds. <i>Journal of Computational Chemistry</i> , 2019, 40, 2473-2481.	1.5	0
1923	Infrared intensity analysis of hydroxyl stretching modes in carboxylic acid dimers by means of the chargeâ€“charge fluxâ€“dipole flux model. <i>Journal of Computational Chemistry</i> , 2019, 40, 2482-2490.	1.5	6
1924	DFT investigation of hostâ€“guest interactions between Î±-Terpineol and Î²-cyclodextrin. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2019, 95, 247-258.	0.9	16
1925	Vibrational spectroscopy of imidazolium-based ionic liquids: A combined MD/DFT study. <i>Journal of Molecular Liquids</i> , 2019, 292, 111282.	2.3	6
1926	H <sub>2</sub> O/Olefinic-I interaction inside a Carbon Nanocage. <i>Journal of the American Chemical Society</i> , 2019, 141, 12928-12938.	6.6	26
1927	Pd(II) Complexes with Chelating Phosphinoferrrocene Diaminocarbene Ligands: Synthesis, Characterization, and Catalytic Use in Pd-Catalyzed Borylation of Aryl Bromides. <i>Organometallics</i> , 2019, 38, 3060-3073.	1.1	13
1928	Relationships between Interaction Energy and Electron Density Properties for Homo Halogen Bonds of the [(A) <sub>n</sub> Yâ€“Xâ€“Z(B) <sub>m</sub> ] Type (X = Cl, Br, I). <i>Molecules</i> , 2019, 24, 2733.	1.7	29
1929	Theoretical calculations of a porous coordination polymer formed by isonicotinylhydrazine, 1,4-benzenedicarboxylic and Co <sup>2+</sup> : electronic properties, lithium doping, and H <sub>2</sub> adsorption studies. <i>Structural Chemistry</i> , 2019, 30, 2369-2377.	1.0	2
1930	Untangling Hydrogen Bond Networks with Ion Mobility Spectrometry and Quantum Chemical Calculations: A Case Study on H <sub>2</sub> XPGG. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5730-5741.	1.2	2

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1932	Experimental and molecular modeling study of a novel arylsulfonamide chalcone. <i>Journal of Molecular Modeling</i> , 2019, 25, 208.	0.8	4
1933	Atoms in Molecules from Alchemical Perturbation Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10073-10082.	1.2	18
1934	Unravelling the Weak Interactions in Binary Clusters of Serotonin and Amino Acid Residues. <i>ChemistrySelect</i> , 2019, 4, 9978-9986.	0.7	4
1935	Structural and Reactivity Analyses of Nitrofurantoin-4-dimethylaminopyridine Salt Using Spectroscopic and Density Functional Theory Calculations. <i>Crystals</i> , 2019, 9, 413.	1.0	7
1936	Hydrogen bonding in the complexes formed by arsine and H-X molecules: A theoretical study. <i>Chemical Physics Letters</i> , 2019, 735, 136767.	1.2	6
1937	Theoretical studies on the bond strength and electron density characteristics in multiple hydrogen bonded arrays. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 93, 107439.	1.3	10
1938	The Na-O bond in sodium fenamate. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 766-774.	0.5	4
1939	Molecular Understanding of Solvents and Glycitein Interaction during Extraction. <i>ACS Omega</i> , 2019, 4, 17823-17829.	1.6	7
1940	A theoretical investigation on the complexes of B3O3H3 with acetylene and its substituted derivatives. <i>Journal of Molecular Modeling</i> , 2019, 25, 332.	0.8	2
1941	Evidence of C-H...O Interactions in the Thiophene:Water Complex. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10406-10417.	1.1	10
1942	Kinetic, Spectroscopic, and DFT Studies of Novel Oxidation of Acetylsalicylic Acid by NaIO4 Using Micro-amount of Os(VIII) As a Homogeneous Catalyst in Alkaline Medium. <i>Russian Journal of Physical Chemistry A</i> , 2019, 93, 2023-2031.	0.1	3
1943	How much do we know about seabird bycatch in pelagic longline fisheries? A simulation study on the potential bias caused by the usually unobserved portion of seabird bycatch. <i>PLoS ONE</i> , 2019, 14, e0220797.	1.1	5
1944	Applications of Cellulose-based Materials in Sustained Drug Delivery Systems. <i>Current Medicinal Chemistry</i> , 2019, 26, 2485-2501.	1.2	120
1945	Hydrogen Bonding versus H...H Interactions in Pillar[n]arenes. <i>ChemistrySelect</i> , 2019, 4, 9354-9359.	0.7	3
1946	TriQuinoline. <i>Nature Communications</i> , 2019, 10, 3820.	5.8	25
1947	Multiscale Computational Study on the Catalytic Mechanism of the Nonmetallo Amidase Maleamate Amidohydrolase (NicF). <i>Journal of Physical Chemistry A</i> , 2019, 123, 7710-7719.	1.1	1
1948	A comparative study of intramolecular hydrogen bond on N-formylformamide derivatives in ground and first singlet excited state: a DFT and TD-DFT study. <i>SN Applied Sciences</i> , 2019, 1, 1.	1.5	1

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1950	A density functional theory study on complexation processes and intermolecular interactions of triptycene-derived oxalixarenes. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	34
1951	Differential uranyl(v) oxo-group bonding between the uranium and metal cations from groups 1, 2, 4, and 12; a high energy resolution X-ray absorption, computational, and synthetic study. <i>Chemical Science</i> , 2019, 10, 9740-9751.	3.7	29
1952	2C <sup>h</sup> 2N square and hexagon interactions: a combined crystallographic data analysis and computational study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21568-21576.	1.3	17
1953	Dealing with Hydrogen Bonding on the Conformational Preference of 1,3-Aminopropanols: Experimental and Molecular Dynamics Approaches. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8583-8594.	1.1	9
1954	A Comprehensive Topological Analysis on a New Bromine-Chalcone with Potential Nonlinear Optical Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8632-8643.	1.1	5
1955	Vibrational spectra, hydrogen bonding interactions and chemical reactivity analysis of nicotinamide-citric acid cocrystals by an experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2019, 43, 15956-15967.	1.4	10
1956	Effect of cluster of protic pyrazolium ionic liquids or epoxides on the cycloaddition of CO <sub>2</sub> . <i>Journal of Molecular Liquids</i> , 2019, 295, 111652.	2.3	4
1957	Pyrene-Based Chemosensor for Picric Acid—Fundamentals to Smartphone Device Design. <i>Analytical Chemistry</i> , 2019, 91, 13244-13250.	3.2	56
1958	Conformational preferences of N-acetyl-N <sup>ε</sup> -methylprolineamide in different media: a <sup>1</sup> H NMR and theoretical investigation. <i>New Journal of Chemistry</i> , 2019, 43, 1757-1763.	1.4	5
1959	<sup>13</sup> C-Hydrogen bonding and aromaticity: a systematic interplay study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 623-630.	1.3	29
1960	Competitive hydrogen-bonding and halogen-bonding interactions in the dimerization of hypobromous acid (HOBr) molecules. <i>Structural Chemistry</i> , 2019, 30, 1335-1341.	1.0	0
1961	Exploiting the Hydrogen Bond Donor/Acceptor Properties of PN-Heterocycles: Selective Anion Receptors for Hydrogen Sulfate. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3934-3938.	7.2	25
1962	Theoretical insights into the metal chelating and antimicrobial properties of the chalcone based Schiff bases. <i>Molecular Simulation</i> , 2019, 45, 636-645.	0.9	19
1963	Computer-Aided Design of Molecularly Imprinted Polymers for Simultaneous Detection of Clenbuterol and Its Metabolites. <i>Polymers</i> , 2019, 11, 17.	2.0	47
1964	From the propargyl alcohol-water complex to the propargyl alcohol dimer: where does the propargyl alcohol-methanol complex fit in?. <i>New Journal of Chemistry</i> , 2019, 43, 3969-3980.	1.4	1
1965	Remarkable shifts of C sp <sup>2</sup> C-H and O-H stretching frequencies and stability of complexes of formic acid with formaldehydes and thioformaldehydes. <i>Journal of Computational Chemistry</i> , 2019, 40, 1387-1400.	1.5	10
1966	Insights into the nature of weak noncovalent interactions in 3-(4-fluorophenyl)-6-(2-fluorophenyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole, a potential bioactive agent: X-ray, QTAIM and molecular docking analysis. <i>Journal of Molecular Structure</i> , 2019, 1183, 331-341.	1.8	9

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1967	A computational study on the characteristics of open-shell H-bonding interaction between carbamic acid (NH <sub>2</sub> COOH) and HO <sub>2</sub> , HOS or HSO radicals. <i>Journal of Molecular Modeling</i> , 2019, 25, 189.	0.8	6
1968	Experimental and theoretical DFT (B3LYP, X3LYP, CAM-B3LYP and M06-2X) study on electronic structure, spectral features, hydrogen bonding and solvent effects of 4-methylthiadiazole-5-carboxylic acid. <i>Molecular Simulation</i> , 2019, 45, 1029-1043.	0.9	33
1969	Exploration of H <sub>2</sub> S capture by alkanolamines. <i>Structural Chemistry</i> , 2019, 30, 2419-2428.	1.0	4
1970	QTAIM, NBO, and NMR studies of hydrogen bonds in capecitabine. <i>Monatshefte für Chemie</i> , 2019, 150, 1267-1274.	0.9	6
1971	Non-covalent loading of ionic liquid-functionalized nanoparticles for bovine serum albumin: experiments and theoretical analysis. <i>RSC Advances</i> , 2019, 9, 19114-19120.	1.7	8
1972	The structure and hydrogen-bond behaviours of binary systems containing ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate and methanol/ethanol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 223, 117312.	2.0	16
1973	Effects of the inter- and intra-molecular hydrogen bonding interactions in forming atmospheric malonic acid-containing clusters. <i>Chemical Physics</i> , 2019, 524, 14-20.	0.9	2
1974	Anion-binding properties of $\pi$ -electron deficient cavity in tetraoxacalix[2]arene[2]triazine by a computational study. <i>Journal of Molecular Liquids</i> , 2019, 288, 111007.	2.3	2
1975	Sulfur as a hydrogen bond donor in the gas phase: Rotational spectroscopic and computational study of 3-mercaptopropionic acid. <i>Journal of Molecular Spectroscopy</i> , 2019, 362, 1-7.	0.4	5
1976	Nitrofurantoin-melamine monohydrate (cocrystal hydrate): Probing the role of H-bonding on the structure and properties using quantum chemical calculations and vibrational spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 221, 117170.	2.0	11
1977	Interplay of weak noncovalent interactions in two conjugated positional isomers: A combined X-ray, optical properties and theoretical investigation. <i>Journal of Molecular Structure</i> , 2019, 1195, 32-42.	1.8	14
1978	Ab initio investigation of cationic water cluster (H <sub>2</sub> O) <sub>+13</sub> via particle swarm optimization algorithm. <i>Theoretical Chemistry Accounts</i> , 2019, 138, 1.	0.5	4
1979	Ten-membered rings as key interaction motifs in folding of desmuramyl di-, tri-, and tetrapeptides. <i>Structural Chemistry</i> , 2019, 30, 743-754.	1.0	1
1980	Thermodynamic, DFT and molecular dynamics studies of intermolecular interactions between 2-methoxyaniline and N- substituted amide mixtures. <i>Chemical Data Collections</i> , 2019, 22, 100241.	1.1	2
1981	Cu(II) and Co(II) coordination solids involving unconventional parallel nitrile( $\pi$ )-nitrile( $\pi$ ) and energetically significant cooperative hydrogen bonding interactions: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2019, 1195, 733-743.	1.8	31
1982	Enhancement of Atmospheric Nucleation by Highly Oxygenated Organic Molecules: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5367-5377.	1.1	10
1983	Experimental, DFT dimeric modeling and AIM study of H-bond-mediated composite vibrational structure of Chelidonic acid. <i>Heliyon</i> , 2019, 5, e01586.	1.4	15
1984	Phosphorene and graphene flakes under the effect of external electric field as an anode material for high-performance lithium-ion batteries: A first-principles study. <i>Computational Materials Science</i> , 2019, 165, 144-153.	1.4	23

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1986	A proton transfer compound template phenylethylamine: Synthesis, a collective experimental and theoretical investigations. Journal of Molecular Structure, 2019, 1191, 183-196.	1.8	50
1987	Proton tautomerism in 2-nitramino-C-nitropyridine derivatives - Experimental and quantum chemical study. Journal of Molecular Structure, 2019, 1186, 317-324.	1.8	3
1988	Hydrogen bonding capabilities of group 14 homologues of HCN and HNC. RSC Advances, 2019, 9, 5937-5941.	1.7	2
1989	Impact of neutral and acidic species on cycloalkenes nucleation. Structural Chemistry, 2019, 30, 1415-1426.	1.0	2
1990	An experimental and theoretical study on 2-hydroxyethylammonium acetate ionic liquid. Journal of Molecular Liquids, 2019, 284, 271-281.	2.3	13
1991	Study of molecular structure and hydrogen bond interactions in dipfluzine-benzoic acid (DIP-BEN) cocrystal using spectroscopic and quantum chemical method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 216, 7-14.	2.0	11
1992	Theoretical investigation of the solubility of some antiemetic drugs. Journal of Molecular Liquids, 2019, 282, 626-632.	2.3	7
1993	Gas sensors based on mass-sensitive transducers part 1: transducers and receptorsâ€”basic understanding. Analytical and Bioanalytical Chemistry, 2019, 411, 1761-1787.	1.9	21
1994	Quantitative and qualitative analyses of intermolecular interactions in neutral/deprotonated aspirin@Î²-CD inclusion complexes: QTAIM and NBO analyses. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	4
1995	Functionalized graphene pieces to trap the insecticide imidacloprid: a theoretical analysis. Journal of Molecular Modeling, 2019, 25, 117.	0.8	10
1996	Spectroscopic (FT-IR, FT-Raman, and <sup>13</sup> C SS-NMR) and quantum chemical investigations to provide structural insights into nitrofurantoin@4-hydroxybenzoic acid cocrystals. New Journal of Chemistry, 2019, 43, 7136-7149.	1.4	6
1997	Chitosan-iron oxide hybrid composite: mechanism of hexavalent chromium removal by central composite design and theoretical calculations. Environmental Science and Pollution Research, 2019, 26, 15973-15988.	2.7	10
1998	Atmospheric Initial Nucleation Containing Carboxylic Acids. Journal of Physical Chemistry A, 2019, 123, 3876-3886.	1.1	9
1999	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. Journal of Physical Chemistry C, 2019, 123, 11850-11859.	1.5	56
2000	The structure of proton-bound Triethylammonia (X@F, Cl) Clusters. Molecular Physics, 2019, 117, 2972-2979.	0.8	2
2001	Effects of methylation in acceptors on the hydrogen bond complexes between 2,2,2-trifluoroethanol and cyclic ethers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 217, 237-246.	2.0	7
2002	The Role of Intramolecular Interactions on the Bioactive Conformation of Epinephrine. Molecular Informatics, 2019, 38, e1800167.	1.4	5

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2004	Anion-adaptive crystalline cationic material for $^{99}\text{TcO}_4^-$ trapping. <i>Nature Communications</i> , 2019, 10, 1532.	5.8	87
2005	Computational study on intermolecular charge transfer complex of 2,2'-bipyridine with picric acid: TD-DFT, NBO and QTAIM analysis. <i>Materials Research Express</i> , 2019, 6, 075104.	0.8	5
2006	Quantum Chemical Modeling of the Structure and H Bonding in Triethanolammonium-Based Protic Ionic Liquids with Sulfonic Acids. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3735-3742.	1.1	9
2007	Effect of external electric field on $\text{C}=\text{X} \cdots \text{Y}$ halogen bonds. <i>Journal of Molecular Modeling</i> , 2019, 25, 57.	0.8	11
2008	Exploiting the Hydrogen Bond Donor/Acceptor Properties of PN-Heterocycles: Selective Anion Receptors for Hydrogen Sulfate. <i>Angewandte Chemie</i> , 2019, 131, 3974-3978.	1.6	6
2009	From glucose to enantiopure morpholino $\beta$ -amino acid: a new tool for stabilizing $\beta$ -turns in peptides. <i>Organic Chemistry Frontiers</i> , 2019, 6, 972-982.	2.3	26
2010	Synthesis and physico-chemical properties of a novel chromate compound with potential biological applications, bis(2-phenylethylammonium) chromate(VI). <i>Journal of Molecular Structure</i> , 2019, 1185, 168-182.	1.8	57
2011	Nature and Strength of $\text{M} \cdots \text{H} \cdots \text{S}$ and $\text{M} \cdots \text{H} \cdots \text{Se}$ ( $\text{M} = \text{Mn, Fe, \& Co}$ ) Hydrogen Bond. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2227-2236.	1.1	23
2012	Experimental and theoretical charge-density analysis of hippuric acid: insight into its binding with human serum albumin. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 750-762.	0.5	3
2013	Formation of large clusters of $\text{CO}_2$ around anions: DFT study reveals cooperative $\text{CO}_2$ adsorption. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23143-23153.	1.3	15
2014	Systematic investigation of hydrogen-bond propensities for informing co-crystal design and assembly. <i>CrystEngComm</i> , 2019, 21, 6048-6055.	1.3	27
2015	Triethylamine-Based Salts: Protic Ionic Liquids or Molecular Complexes?. <i>Journal of Physical Chemistry B</i> , 2019, 123, 10794-10806.	1.2	23
2016	Diethylamine-based ionic liquids: quantum chemical calculations and experiment. <i>Russian Chemical Bulletin</i> , 2019, 68, 2009-2019.	0.4	8
2017	Molecular interaction between MeOH and genistein during soy extraction. <i>RSC Advances</i> , 2019, 9, 39170-39179.	1.7	8
2018	A molecular understanding of the interaction of typical aromatic acids with common aerosol nucleation precursors and their atmospheric implications. <i>RSC Advances</i> , 2019, 9, 36171-36181.	1.7	15
2019	Combined quantum mechanics/molecular mechanics (QM/MM) methods to understand the charge density distribution of estrogens in the active site of estrogen receptors. <i>RSC Advances</i> , 2019, 9, 40758-40771.	1.7	5
2020	Experimental and theoretical charge density, intermolecular interactions and electrostatic properties of metronidazole. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 942-953.	0.5	10



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2021	Hydrogen bond interactions of dopamine hydrochloride with urea. <i>Physics and Chemistry of Liquids</i> , 2019, 57, 746-754.	0.4	4
2022	Carbene triel bonds between TrR 3 (Trâ€‰%o=â€‰%B, Al) and Nâ€‰heterocyclic carbenes. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25867.	1.0	27
2023	Acylguanidine-BACE1 complex: Insights of intermolecular interactions and dynamics. <i>Journal of Theoretical Biology</i> , 2019, 464, 33-49.	0.8	11
2024	Spectroscopic and electronic structure characterization of hydrogen bonding in 2-Bromohydroquinone. <i>Journal of Molecular Structure</i> , 2019, 1181, 71-82.	1.8	8
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2289	Non-Covalent Forces in Naphthazarin <sup>+</sup> Cooperativity or Competition in the Light of Theoretical Approaches. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8033.	1.8	6
2290	A combined experimental and theoretical study on diglyme <sup>+</sup> -alkanol liquid mixtures. <i>Journal of Molecular Liquids</i> , 2021, 334, 116048.	2.3	1

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2464	Tracing electron density changes in langbeinite under pressure. <i>IUCr</i> , 2022, 9, 146-162.	1.0	4
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