Clemence Corminboeuf

List of Publications by Year
in descending order

139 papers	5,910 citations	70961 41 h-index	85405 71 g-index
146 all docs	146 docs citations	146 times ranked	7168 citing authors

#	Article	IF	Citations
1	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. Topics in Catalysis, 2022, 65, 289-295.	1.3	3
2	Heteroatom oxidation controls singletâ€“triplet energy splitting in singlet fission building blocks. Chemical Communications, 2022, 58, 1338-1341.	2.2	6
3	SPA^HM: the spectrum of approximated Hamiltonian matrices representations. , 2022, 1, 286-294.		7
4	Local Kernel Regression and Neural Network Approaches to the Conformational Landscapes of Oligopeptides. Journal of Chemical Theory and Computation, 2022, 18, 1467-1479.	2.3	8
5	Machine intelligence for chemical reaction space. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	30
6	Genetic Optimization of Homogeneous Catalysts. Chemistry Methods, 2022, 2, .	1.8	14
7	Assessing the persistence of chalcogen bonds in solution with neural network potentials. Journal of Chemical Physics, 2022, 156, 154112.	1.2	6
8	Mapping Active Site Geometry to Activity in Immobilized Frustrated Lewis Pair Catalysts. Angewandte Chemie - International Edition, 2022, 61, .	7.2	5
9	Optimizing the Thermodynamics and Kinetics of the Triplet-Pair Dissociation in Donorâ€“Acceptor Copolymers for Intramolecular Singlet Fission. Chemistry of Materials, 2022, 34, 4115-4121.	3.2	6
10	Mapping Catalystâ€“Solvent Interplay in Competing Carboamination/Cyclopropanation Reactions. Chemistry - A European Journal, 2022, , .	1.7	1
11	Modular Synthesis of Benzocyclobutenes via Pd(II)-Catalyzed Oxidative [2+2] Annulation of Arylboronic Acids with Alkenes. Journal of the American Chemical Society, 2022, 144, 8920-8926.	6.6	9
12	The (not so) simple prediction of enantioselectivity â€“ a pipeline for high-fidelity computations. Chemical Science, 2022, 13, 6858-6864.	3.7	6
13	Donorâ€“Acceptorâ€“Donor â€œHot Excitonâ€•Triads for High Reverse Intersystem Crossing in OLEDs. Advanced Optical Materials, 2022, 10, .	3.6	7
14	Harvesting the fragment-based nature of bifunctional organocatalysts to enhance their activity. Organic Chemistry Frontiers, 2022, 9, 4041-4051.	2.3	3
15	How Robust Is the Reversible Steric Shielding Strategy for Photoswitchable Organocatalysts?. Journal of Organic Chemistry, 2022, 87, 8849-8857.	1.7	3
16	Structureâ€“Property Relationships in Bithiophenes with Hydrogenâ€Bonded Substituents. Chemistry - A European Journal, 2021, 27, 3348-3360.	1.7	5
17	Helical electronic transitions of spiroconjugated molecules. Chemical Communications, 2021, 57, 6408-6411.	2.2	13
18	The Genesis of Molecular Volcano Plots. Accounts of Chemical Research, 2021, 54, 1107-1117.	7.6	54

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19	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2021, 33, 2567-2575.	3.2	14
20	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4
21	Impact of quantum-chemical metrics on the machine learning prediction of electron density. Journal of Chemical Physics, 2021, 155, 024107.	1.2	3
22	Tuning the Ï€âˆ—Accepting Properties of Mesoionic Carbenes: A Combined Computational and Experimental Study. Chemistry - A European Journal, 2021, 27, 11983-11988.	1.7	10
23	Pushing the Limits of the Donorâ€“Acceptor Copolymer Strategy for Intramolecular Singlet Fission. Journal of Physical Chemistry Letters, 2021, 12, 7270-7277.	2.1	5
24	Is a Single Conformer Sufficient to Describe the Reorganization Energy of Amorphous Organic Transport Materials?. Journal of Physical Chemistry C, 2021, 125, 17355-17362.	1.5	6
25	Methoxycyclization of 1,5â€Enynes by Coinage Metal Catalysts: Is Gold Always Superior?. Helvetica Chimica Acta, 2021, 104, e2100134.	1.0	2
26	Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. Chemical Science, 2021, 12, 6879-6889.	3.7	54
27	Tuning the Thermal Stability and Photoisomerization of Azoheteroarenes through Macrocycle Strain**. Chemistry - A European Journal, 2021, 27, 419-426.	1.7	12
28	Doped but Stable: Spirobisacridine Hole Transporting Materials for Hysteresis-Free and Stable Perovskite Solar Cells. Journal of the American Chemical Society, 2020, 142, 1792-1800.	6.6	39
29	Data-powered augmented volcano plots for homogeneous catalysis. Chemical Science, 2020, 11, 12070-12080.	3.7	23
30	The Photoisomerization Pathway(s) of Pushâ€“Pull Phenylazoheteroarenes**. Chemistry - A European Journal, 2020, 26, 14724-14729.	1.7	6
31	Designing Singlet Fission Candidates from Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2020, 32, 6515-6524.	3.2	27
32	Optical gap and fundamental gap of oligoynes and carbyne. Nature Communications, 2020, 11, 4797.	5.8	28
33	Probing Substrate Scope with Molecular Volcanoes. Organic Letters, 2020, 22, 7936-7941.	2.4	12
34	Optical absorption properties of metalâ€“organic frameworks: solid state versus molecular perspective. Physical Chemistry Chemical Physics, 2020, 22, 19512-19521.	1.3	14
35	FB-ECDA: Fragment-based Electronic Coupling Decomposition Analysis for Organic Amorphous Semiconductors. Journal of Physical Chemistry A, 2020, 124, 10624-10634.	1.1	2
36	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donorâ€“Acceptor Copolymers. Journal of Physical Chemistry Letters, 2020, 11, 9788-9794.	2.1	11

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37	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. Chimia, 2020, 74, 232-236.	0.3	9
38	Machine learning models of the energy curvature vs particle number for optimal tuning of long-range corrected functionals. Journal of Chemical Physics, 2020, 152, 154103.	1.2	12
39	FB-REDA: fragment-based decomposition analysis of the reorganization energy for organic semiconductors. Physical Chemistry Chemical Physics, 2020, 22, 11881-11890.	1.3	10
40	Data-Driven Advancement of Homogeneous Nickel Catalyst Activity for Aryl Ether Cleavage. ACS Catalysis, 2020, 10, 7021-7031.	5.5	40
41	Simulating Solvation and Acidity in Complex Mixtures with First-Principles Accuracy: The Case of CH₃SO₃H and H₂O₂ in Phenol. Journal of Chemical Theory and Computation, 2020, 16, 5139-5149.	2.3	26
42	Hamiltonian-Reservoir Replica Exchange and Machine Learning Potentials for Computational Organic Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 3084-3094.	2.3	16
43	Crystallization and Organic Fieldâ€Effect Transistor Performance of a Hydrogenâ€Bonded Quaterthiophene. Chemistry - A European Journal, 2020, 26, 10265-10275.	1.7	5
44	Balancing Density Functional Theory Interaction Energies in Charged Dimers Precursors to Organic Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3530-3542.	2.3	2
45	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie, 2020, 132, 15013-15019.	1.6	9
46	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie - International Edition, 2020, 59, 14903-14909.	7.2	85
47	Correlation between Optical Activity and the Helical Molecular Orbitals of Allene and Cumulenes. Organic Letters, 2020, 22, 8028-8033.	2.4	9
48	Learning on-top: Regressing the on-top pair density for real-space visualization of electron correlation. Journal of Chemical Physics, 2020, 153, 204111.	1.2	10
49	Tuning the structure, reactivity and magnetic communication of nitride-bridged uranium complexes with the ancillary ligands. Chemical Science, 2019, 10, 8840-8849.	3.7	26
50	Open-Shell Nonbenzenoid Nanographenes Containing Two Pairs of Pentagonal and Heptagonal Rings. Journal of the American Chemical Society, 2019, 141, 12011-12020.	6.6	112
51	Dual-Facet Mechanism in Copper Nanocubes for Electrochemical CO₂ Reduction into Ethylene. Journal of Physical Chemistry Letters, 2019, 10, 4259-4265.	2.1	52
52	Mechanistic Study on the Photogeneration of Hydrogen by Decamethylruthenocene. Chemistry - A European Journal, 2019, 25, 12769-12779.	1.7	9
53	Getting the Right Twist: Influence of Donorâ€“Acceptor Dihedral Angle on Exciton Kinetics and Singletâ€“Triplet Gap in Deep Blue Thermally Activated Delayed Fluorescence Emitter. Journal of Physical Chemistry C, 2019, 123, 27778-27784.	1.5	40
54	Exploring chemical space in the search for improved azoheteroarene-based photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 20782-20790.	1.3	10

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55	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	3.7	92
56	Insights into Reaction Intermediates to Predict Synthetic Pathways for Shape-Controlled Metal Nanocrystals. Journal of the American Chemical Society, 2019, 141, 16312-16322.	6.6	47
57	The influence of external electric fields on charge reorganization energy in organic semiconductors. Chemical Communications, 2019, 55, 2384-2387.	2.2	9
58	Topology-Driven Single-Molecule Conductance of Carbon Nanothreads. Journal of Physical Chemistry Letters, 2019, 10, 825-830.	2.1	18
59	Synthesis of aminyl biradicals by base-induced Csp³â€“Csp³ coupling of cationic azo dyes. Chemical Science, 2019, 10, 5719-5724.	3.7	30
60	Activity-Based Screening of Homogeneous Catalysts through the Rapid Assessment of Theoretically Derived Turnover Frequencies. ACS Catalysis, 2019, 9, 5716-5725.	5.5	48
61	Data Mining the Câ^'C Crossâ€Coupling Genome. ChemCatChem, 2019, 11, 4096-4107.	1.8	15
62	DORI Reveals the Influence of Noncovalent Interactions on Covalent Bonding Patterns in Molecular Crystals Under Pressure. Journal of Physical Chemistry Letters, 2019, 10, 1482-1488.	2.1	15
63	Mechanisms of fluorescence quenching in prototypical aggregation-induced emission systems: excited state dynamics with TD-DFTB. Physical Chemistry Chemical Physics, 2019, 21, 9026-9035.	1.3	28
64	An Unconventional Iron Nickel Catalyst for the Oxygen Evolution Reaction. ACS Central Science, 2019, 5, 558-568.	5.3	263
65	Multiarm and Substituent Effects on Charge Transport of Organic Hole Transport Materials. Chemistry of Materials, 2019, 31, 6605-6614.	3.2	21
66	Quantum Chemistry Meets Machine Learning. Chimia, 2019, 73, 983.	0.3	8
67	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	5.3	178
68	The role of bridging ligands in dinitrogen reduction and functionalization by uranium multimetallic complexes. Nature Chemistry, 2019, 11, 154-160.	6.6	100
69	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
70	Noncovalent Molecular Electronics. Journal of Physical Chemistry Letters, 2018, 9, 2298-2304.	2.1	14
71	How does alkyl chain length modify the properties of triphenylamine-based hole transport materials?. Journal of Materials Chemistry C, 2018, 6, 960-965.	2.7	23
72	How do London Dispersion Interactions Impact the Photochemical Processes of Molecular Switches?. Journal of Physical Chemistry Letters, 2018, 9, 464-470.	2.1	22

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73	Analyzing Fluxional Molecules Using DORI. Journal of Chemical Theory and Computation, 2018, 14, 2370-2379.	2.3	5
74	Improving the Thermodynamic Profiles of Prospective Suzukiâ€“Miyaura Crossâ€Coupling Catalysts by Altering the Electrophilic Coupling Component. ChemCatChem, 2018, 10, 1592-1597.	1.8	21
75	On the Generality of Molecular Volcano Plots. ChemCatChem, 2018, 10, 1586-1591.	1.8	29
76	Unraveling Metal/Pincer Ligand Effects in the Catalytic Hydrogenation of Carbon Dioxide to Formate. Organometallics, 2018, 37, 4568-4575.	1.1	32
77	Restriction Enzyme Analysis of Double-Stranded DNA on Pristine Single-Walled Carbon Nanotubes. ACS Applied Materials & Interfaces, 2018, 10, 37386-37395.	4.0	15
78	Read between the Molecules: Computational Insights into Organic Semiconductors. Journal of the American Chemical Society, 2018, 140, 16370-16386.	6.6	79
79	Exploring the Limitation of Molecular Water Oxidation Catalysts. Journal of Physical Chemistry C, 2018, 122, 12404-12412.	1.5	37
80	Fine-tuned organic photoredox catalysts for fragmentation-alkynylation cascades of cyclic oxime ethers. Chemical Science, 2018, 9, 5883-5889.	3.7	141
81	Infrared Spectroscopy as a Probe of Electronic Energy Transfer. Journal of Physical Chemistry Letters, 2018, 9, 3217-3223.	2.1	10
82	Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction. Helvetica Chimica Acta, 2018, 101, e1800107.	1.0	19
83	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. Chemical Science, 2018, 9, 7069-7077.	3.7	154
84	Steric â€œattractionâ€• not by dispersion alone. Beilstein Journal of Organic Chemistry, 2018, 14, 1482-1490.	1.3	23
85	Nickel pincer model of the active site of lactate racemase involves ligand participation in hydride transfer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1242-1245.	3.3	39
86	Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations. Chemical Communications, 2017, 53, 2423-2426.	2.2	6
87	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. Angewandte Chemie - International Edition, 2017, 56, 2324-2327.	7.2	24
88	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. Angewandte Chemie, 2017, 129, 2364-2367.	1.6	6
89	Synthesis and characterization of semiaromatic polyamides comprising benzofurobenzofuran repeating units. Polymer Chemistry, 2017, 8, 2197-2209.	1.9	14
90	Heterotetracenes: Flexible Synthesis and in Silico Assessment of the Holeâ€Transport Properties. Chemistry - A European Journal, 2017, 23, 8058-8065.	1.7	26

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91	Fluorescence Quenching in BODIPY Dyes: The Role of Intramolecular Interactions and Charge Transfer. Helvetica Chimica Acta, 2017, 100, e1700093.	1.0	45
92	Perspective: Found in translation: Quantum chemical tools for grasping non-covalent interactions. Journal of Chemical Physics, 2017, 146, 120901.	1.2	90
93	Charge transport in highly ordered organic nanofibrils: lessons from modelling. Journal of Materials Chemistry C, 2017, 5, 350-361.	2.7	22
94	Salt-induced thermochromism of a conjugated polyelectrolyte. Physical Chemistry Chemical Physics, 2017, 19, 28853-28866.	1.3	12
95	A Î²-Carbon elimination strategy for convenient in situ access to cyclopentadienyl metal complexes. Chemical Science, 2017, 8, 7174-7179.	3.7	53
96	A Rising Star: Truxene as a Promising Hole Transport Material in Perovskite Solar Cells. Journal of Physical Chemistry C, 2017, 121, 21729-21739.	1.5	32
97	A Generalized Picture of Câ€“C Cross-Coupling. ACS Catalysis, 2017, 7, 5643-5653.	5.5	68
98	Guidelines and diagnostics for charge carrier tuning in thiophene-based wires. Physical Chemistry Chemical Physics, 2017, 19, 23254-23259.	1.3	10
99	Photochromic Torsional Switch (PTS): a light-driven actuator for the dynamic tuning of Ï€-conjugation extension. Chemical Science, 2017, 8, 361-365.	3.7	15
100	Implications of Charge Penetration for Heteroatom-Containing Organic Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 5198-5204.	2.1	31
101	Low-Lying Ï€Ï€* States of Heteroaromatic Molecules: A Challenge for Excited State Methods. Journal of Chemical Theory and Computation, 2016, 12, 2652-2660.	2.3	56
102	Rationalizing fluorescence quenching in meso-BODIPY dyes. Physical Chemistry Chemical Physics, 2016, 18, 32668-32672.	1.3	48
103	Neutral Aminyl Radicals Derived from Azoimidazolium Dyes. Journal of the American Chemical Society, 2016, 138, 15126-15129.	6.6	40
104	Visualizing and Quantifying Interactions in the Excited State. Chemistry - A European Journal, 2016, 22, 18442-18449.	1.7	22
105	Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots. Chemical Science, 2016, 7, 5723-5735.	3.7	65
106	Beyond static structures: Putting forth REMD as a tool to solve problems in computational organic chemistry. Journal of Computational Chemistry, 2016, 37, 83-92.	1.5	27
107	How does tetraphenylethylene relax from its excited states?. Physical Chemistry Chemical Physics, 2016, 18, 11606-11609.	1.3	86
108	Exploiting Dispersion-Driven Aggregators as a Route to New One-Dimensional Organic Nanowires. Journal of Physical Chemistry Letters, 2015, 6, 4422-4428.	2.1	10

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109	Theory and practice of uncommon molecular electronic configurations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 440-459.	6.2	95
110	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. Journal of Chemical Physics, 2015, 143, 224107.	1.2	19
111	A fast chargeâ€Dependent atomâ€pairwise dispersion correction for DFTB3. International Journal of Quantum Chemistry, 2015, 115, 1265-1272.	1.0	16
112	Toward Functional Typeâ€...III [Fe]â€Hydrogenase Biomimics for H₂ Activation: Insights from Computation. Chemistry - A European Journal, 2015, 21, 3987-3996.	1.7	20
113	Communication: A new class of non-empirical explicit density functionals on the third rung of Jacobâ€™s ladder. Journal of Chemical Physics, 2015, 143, 111105.	1.2	13
114	Local hybrid functionals with orbital-free mixing functions and balanced elimination of self-interaction error. Journal of Chemical Physics, 2015, 142, 074112.	1.2	31
115	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. Physical Chemistry Chemical Physics, 2015, 17, 14719-14730.	1.3	57
116	Linear scaling relationships and volcano plots in homogeneous catalysis â€“ revisiting the Suzuki reaction. Chemical Science, 2015, 6, 6754-6761.	3.7	98
117	Exploration of zeroth-order wavefunctions and energies as a first step toward intramolecular symmetry-adapted perturbation theory. Journal of Chemical Physics, 2014, 140, 154107.	1.2	15
118	How important is self-consistency for the dDsC density dependent dispersion correction?. Journal of Chemical Physics, 2014, 140, 18A516.	1.2	24
119	Functional carbon nanosheets prepared from hexayne amphiphile monolayers at room temperature. Nature Chemistry, 2014, 6, 468-476.	6.6	97
120	Adjusting the Local Arrangement of Ï€-Stacked Oligothiophenes through Hydrogen Bonds: A Viable Route to Promote Charge Transfer. Journal of Physical Chemistry Letters, 2014, 5, 2320-2324.	2.1	22
121	Ligandâ€Controlled Regiodivergent Pathways of Rhodium(III)â€Catalyzed Dihydroisoquinolone Synthesis: Experimental and Computational Studies of Different Cyclopentadienyl Ligands. Chemistry - A European Journal, 2014, 20, 15409-15418.	1.7	120
122	Simultaneous Visualization of Covalent and Noncovalent Interactions Using Regions of Density Overlap. Journal of Chemical Theory and Computation, 2014, 10, 3745-3756.	2.3	177
123	Minimizing Density Functional Failures for Non-Covalent Interactions Beyond van der Waals Complexes. Accounts of Chemical Research, 2014, 47, 3217-3224.	7.6	51
124	Hierarchically Structured Microfibers of â€œSingle Stackâ€•Perylene Bisimide and Quaterthiophene Nanowires. ACS Nano, 2013, 7, 8498-8508.	7.3	88
125	A ratiometric fluorescence sensor for caffeine. Organic and Biomolecular Chemistry, 2012, 10, 7487.	1.5	19
126	Biphasic water splitting by osmocene. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11558-11563.	3.3	41

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127	Exploring the Limits of Density Functional Approximations for Interaction Energies of Molecular Precursors to Organic Electronics. Journal of Chemical Theory and Computation, 2012, 8, 4305-4316.	2.3	38
128	Quantification of â€œfuzzyâ€•chemical concepts: a computational perspective. Chemical Society Reviews, 2012, 41, 4671.	18.7	108
129	Why are the Interaction Energies of Charge-Transfer Complexes Challenging for DFT?. Journal of Chemical Theory and Computation, 2012, 8, 1629-1640.	2.3	153
130	Dispersion-Corrected Energy Decomposition Analysis for Intermolecular Interactions Based on the BLW and dDXDM Methods. Journal of Physical Chemistry A, 2011, 115, 5467-5477.	1.1	43
131	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. Journal of Chemical Theory and Computation, 2011, 7, 3567-3577.	2.3	400
132	A Density Dependent Dispersion Correction. Chimia, 2011, 65, 240.	0.3	40
133	A generalized-gradient approximation exchange hole model for dispersion coefficients. Journal of Chemical Physics, 2011, 134, 044117.	1.2	270
134	Oxygen and proton reduction by decamethylferrocene in non-aqueous acidic media. Chemical Communications, 2010, 46, 2918.	2.2	59
135	A System-Dependent Density-Based Dispersion Correction. Journal of Chemical Theory and Computation, 2010, 6, 1990-2001.	2.3	133
136	Why Are (NN₂)Ni Pincer Complexes Active for Alkylâ''Alkyl Coupling: Î²-H Elimination Is Kinetically Accessible but Thermodynamically Uphill. Organometallics, 2010, 29, 3686-3689.	1.1	76
137	Unified Inter- and Intramolecular Dispersion Correction Formula for Generalized Gradient Approximation Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2950-2958.	2.3	76
138	Can five-membered Te2N2S rings be considered aromatic?. Structural Chemistry, 2007, 18, 841-847.	1.0	3
139	Mapping Active Site Geometry to Activity in Immobilized Frustrated Lewis Pair Catalysts. Angewandte Chemie, 0, , .	1.6	3