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	Comprehensive Benchmarking of a Density-Dependent Dispersion Correction. Journal of Chemical Theory and Computation, 2011, 7, 3567-3577.	2.3	400
2	A generalized-gradient approximation exchange hole model for dispersion coefficients. Journal of Chemical Physics, 2011, 134, 044117.	1.2	270
3	An Unconventional Iron Nickel Catalyst for the Oxygen Evolution Reaction. ACS Central Science, 2019, 5, 558-568.	5.3	263
4	i-PI 2.0: A universal force engine for advanced molecular simulations. Computer Physics Communications, 2019, 236, 214-223.	3.0	220
5	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	5.3	178
6	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
7	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. Chemical Science, 2018, 9, 7069-7077.	3.7	154
8	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
9	Fine-tuned organic photoredox catalysts for fragmentation-alkynylation cascades of cyclic oxime ethers. Chemical Science, 2018, 9, 5883-5889.	3.7	141
10	A System-Dependent Density-Based Dispersion Correction. Journal of Chemical Theory and Computation, 2010, 6, 1990-2001.	2.3	133
11	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
12	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
13	Quantification of â€œfuzzyâ€•chemical concepts: a computational perspective. Chemical Society Reviews, 2012, 41, 4671.	18.7	108
14	The role of bridging ligands in dinitrogen reduction and functionalization by uranium multimetallic complexes. Nature Chemistry, 2019, 11, 154-160.	6.6	100
15	Linear scaling relationships and volcano plots in homogeneous catalysis â€“ revisiting the Suzuki reaction. Chemical Science, 2015, 6, 6754-6761.	3.7	98
16	Functional carbon nanosheets prepared from hexayne amphiphile monolayers at room temperature. Nature Chemistry, 2014, 6, 468-476.	6.6	97
17	Theory and practice of uncommon molecular electronic configurations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 440-459.	6.2	95
18	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	3.7	92

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19	Perspective: Found in translation: Quantum chemical tools for grasping non-covalent interactions. Journal of Chemical Physics, 2017, 146, 120901.	1.2	90
20	Hierarchically Structured Microfibers of â€œSingle Stackâ€•Perylene Bisimide and Quaterthiophene Nanowires. ACS Nano, 2013, 7, 8498-8508.	7.3	88
21	How does tetraphenylethylene relax from its excited states?. Physical Chemistry Chemical Physics, 2016, 18, 11606-11609.	1.3	86
22	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie - International Edition, 2020, 59, 14903-14909.	7.2	85
23	Read between the Molecules: Computational Insights into Organic Semiconductors. Journal of the American Chemical Society, 2018, 140, 16370-16386.	6.6	79
24	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
25	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
26	A Generalized Picture of Câ€“C Cross-Coupling. ACS Catalysis, 2017, 7, 5643-5653.	5.5	68
27	Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots. Chemical Science, 2016, 7, 5723-5735.	3.7	65
28	Oxygen and proton reduction by decamethylferrocene in non-aqueous acidic media. Chemical Communications, 2010, 46, 2918.	2.2	59
29	Excited state dynamics of thiophene and bithiophene: new insights into theoretically challenging systems. Physical Chemistry Chemical Physics, 2015, 17, 14719-14730.	1.3	57
30	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
31	The Genesis of Molecular Volcano Plots. Accounts of Chemical Research, 2021, 54, 1107-1117.	7.6	54
32	Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. Chemical Science, 2021, 12, 6879-6889.	3.7	54
33	A Î²-Carbon elimination strategy for convenient in situ access to cyclopentadienyl metal complexes. Chemical Science, 2017, 8, 7174-7179.	3.7	53
34	Dual-Facet Mechanism in Copper Nanocubes for Electrochemical CO₂ Reduction into Ethylene. Journal of Physical Chemistry Letters, 2019, 10, 4259-4265.	2.1	52
35	Minimizing Density Functional Failures for Non-Covalent Interactions Beyond van der Waals Complexes. Accounts of Chemical Research, 2014, 47, 3217-3224.	7.6	51
36	Rationalizing fluorescence quenching in meso-BODIPY dyes. Physical Chemistry Chemical Physics, 2016, 18, 32668-32672.	1.3	48

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37	Activity-Based Screening of Homogeneous Catalysts through the Rapid Assessment of Theoretically Derived Turnover Frequencies. ACS Catalysis, 2019, 9, 5716-5725.	5.5	48
38	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
39	Fluorescence Quenching in BODIPY Dyes: The Role of Intramolecular Interactions and Charge Transfer. Helvetica Chimica Acta, 2017, 100, e1700093.	1.0	45
40	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
41	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
42	A Density Dependent Dispersion Correction. Chimia, 2011, 65, 240.	0.3	40
43	Neutral Aminyl Radicals Derived from Azoimidazolium Dyes. Journal of the American Chemical Society, 2016, 138, 15126-15129.	6.6	40
44	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
45	Data-Driven Advancement of Homogeneous Nickel Catalyst Activity for Aryl Ether Cleavage. ACS Catalysis, 2020, 10, 7021-7031.	5.5	40
46	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
47	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
48	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
49	Exploring the Limitation of Molecular Water Oxidation Catalysts. Journal of Physical Chemistry C, 2018, 122, 12404-12412.	1.5	37
50	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
51	Unraveling Metal/Pincer Ligand Effects in the Catalytic Hydrogenation of Carbon Dioxide to Formate. Organometallics, 2018, 37, 4568-4575.	1.1	32
52	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
53	Implications of Charge Penetration for Heteroatom-Containing Organic Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 5198-5204.	2.1	31
54	Synthesis of aminyl biradicals by base-induced Csp³â€“Csp³ coupling of cationic azo dyes. Chemical Science, 2019, 10, 5719-5724.	3.7	30

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55	Machine intelligence for chemical reaction space. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	30
56	On the Generality of Molecular Volcano Plots. ChemCatChem, 2018, 10, 1586-1591.	1.8	29
57	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
58	Optical gap and fundamental gap of oligoynes and carbyne. Nature Communications, 2020, 11, 4797.	5.8	28
59	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
60	Designing Singlet Fission Candidates from Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2020, 32, 6515-6524.	3.2	27
61	Heterotetracenes: Flexible Synthesis and in Silico Assessment of the Holeâ€Transport Properties. Chemistry - A European Journal, 2017, 23, 8058-8065.	1.7	26
62	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
63	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
64	How important is self-consistency for the dDsC density dependent dispersion correction?. Journal of Chemical Physics, 2014, 140, 18A516.	1.2	24
65	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. Angewandte Chemie - International Edition, 2017, 56, 2324-2327.	7.2	24
66	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
67	Steric â€œattractionâ€• not by dispersion alone. Beilstein Journal of Organic Chemistry, 2018, 14, 1482-1490.	1.3	23
68	Data-powered augmented volcano plots for homogeneous catalysis. Chemical Science, 2020, 11, 12070-12080.	3.7	23
69	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
70	Visualizing and Quantifying Interactions in the Excited State. Chemistry - A European Journal, 2016, 22, 18442-18449.	1.7	22
71	Charge transport in highly ordered organic nanofibrils: lessons from modelling. Journal of Materials Chemistry C, 2017, 5, 350-361.	2.7	22
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	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
74	Multiarm and Substituent Effects on Charge Transport of Organic Hole Transport Materials. Chemistry of Materials, 2019, 31, 6605-6614.	3.2	21
75	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
76	A ratiometric fluorescence sensor for caffeine. Organic and Biomolecular Chemistry, 2012, 10, 7487.	1.5	19
77	Intramolecular symmetry-adapted perturbation theory with a single-determinant wavefunction. Journal of Chemical Physics, 2015, 143, 224107.	1.2	19
78	Expedited Screening of Active and Regioselective Catalysts for the Hydroformylation Reaction. Helvetica Chimica Acta, 2018, 101, e1800107.	1.0	19
79	Topology-Driven Single-Molecule Conductance of Carbon Nanothreads. Journal of Physical Chemistry Letters, 2019, 10, 825-830.	2.1	18
80	A fast chargeâ€Dependent atomâ€pairwise dispersion correction for DFTB3. International Journal of Quantum Chemistry, 2015, 115, 1265-1272.	1.0	16
81	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
82	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
83	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
84	Restriction Enzyme Analysis of Double-Stranded DNA on Pristine Single-Walled Carbon Nanotubes. ACS Applied Materials & Interfaces, 2018, 10, 37386-37395.	4.0	15
85	Data Mining the Câ^'C Crossâ€Coupling Genome. ChemCatChem, 2019, 11, 4096-4107.	1.8	15
86	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
87	Synthesis and characterization of semiaromatic polyamides comprising benzofurobenzofuran repeating units. Polymer Chemistry, 2017, 8, 2197-2209.	1.9	14
88	Noncovalent Molecular Electronics. Journal of Physical Chemistry Letters, 2018, 9, 2298-2304.	2.1	14
89	Optical absorption properties of metalâ€“organic frameworks: solid state versus molecular perspective. Physical Chemistry Chemical Physics, 2020, 22, 19512-19521.	1.3	14
90	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2021, 33, 2567-2575.	3.2	14

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91	Genetic Optimization of Homogeneous Catalysts. Chemistry Methods, 2022, 2, .	1.8	14
92	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
93	Helical electronic transitions of spiroconjugated molecules. Chemical Communications, 2021, 57, 6408-6411.	2.2	13
94	Salt-induced thermochromism of a conjugated polyelectrolyte. Physical Chemistry Chemical Physics, 2017, 19, 28853-28866.	1.3	12
95	Probing Substrate Scope with Molecular Volcanoes. Organic Letters, 2020, 22, 7936-7941.	2.4	12
96	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
97	Tuning the Thermal Stability and Photoisomerization of Azoheteroarenes through Macrocycle Strain**. Chemistry - A European Journal, 2021, 27, 419-426.	1.7	12
98	Direct, Mediated, and Delayed Intramolecular Singlet Fission Mechanism in Donorâ€“Acceptor Copolymers. Journal of Physical Chemistry Letters, 2020, 11, 9788-9794.	2.1	11
99	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
100	Guidelines and diagnostics for charge carrier tuning in thiophene-based wires. Physical Chemistry Chemical Physics, 2017, 19, 23254-23259.	1.3	10
101	Infrared Spectroscopy as a Probe of Electronic Energy Transfer. Journal of Physical Chemistry Letters, 2018, 9, 3217-3223.	2.1	10
102	Exploring chemical space in the search for improved azoheteroarene-based photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 20782-20790.	1.3	10
103	FB-REDA: fragment-based decomposition analysis of the reorganization energy for organic semiconductors. Physical Chemistry Chemical Physics, 2020, 22, 11881-11890.	1.3	10
104	Tuning the Ï€â€Accepting Properties of Mesoionic Carbenes: A Combined Computational and Experimental Study. Chemistry - A European Journal, 2021, 27, 11983-11988.	1.7	10
105	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
106	Mechanistic Study on the Photogeneration of Hydrogen by Decamethylruthenocene. Chemistry - A European Journal, 2019, 25, 12769-12779.	1.7	9
107	The influence of external electric fields on charge reorganization energy in organic semiconductors. Chemical Communications, 2019, 55, 2384-2387.	2.2	9
108	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. Chimia, 2020, 74, 232-236.	0.3	9

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109	Direct Observation of Aggregationâ€Induced Emission Mechanism. Angewandte Chemie, 2020, 132, 15013-15019.	1.6	9
110	Correlation between Optical Activity and the Helical Molecular Orbitals of Allene and Cumulenes. Organic Letters, 2020, 22, 8028-8033.	2.4	9
111	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
112	Quantum Chemistry Meets Machine Learning. Chimia, 2019, 73, 983.	0.3	8
113	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
114	SPA^HM: the spectrum of approximated Hamiltonian matrices representations. , 2022, 1, 286-294.		7
115	Donorâ€“Acceptorâ€“Donor â€œHot Excitonâ€•Triads for High Reverse Intersystem Crossing in OLEDs. Advanced Optical Materials, 2022, 10, .	3.6	7
116	Enhancing the power conversion efficiency of dye-sensitized solar cells via molecular plasmon-like excitations. Chemical Communications, 2017, 53, 2423-2426.	2.2	6
117	Photoproduction of Hydrogen by Decamethylruthenocene Combined with Electrochemical Recycling. Angewandte Chemie, 2017, 129, 2364-2367.	1.6	6
118	The Photoisomerization Pathway(s) of Pushâ€“Pull Phenylazoheteroarenes**. Chemistry - A European Journal, 2020, 26, 14724-14729.	1.7	6
119	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
120	Heteroatom oxidation controls singletâ€“triplet energy splitting in singlet fission building blocks. Chemical Communications, 2022, 58, 1338-1341.	2.2	6
121	Assessing the persistence of chalcogen bonds in solution with neural network potentials. Journal of Chemical Physics, 2022, 156, 154112.	1.2	6
122	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
123	The (not so) simple prediction of enantioselectivity â€“ a pipeline for high-fidelity computations. Chemical Science, 2022, 13, 6858-6864.	3.7	6
124	Analyzing Fluxional Molecules Using DORI. Journal of Chemical Theory and Computation, 2018, 14, 2370-2379.	2.3	5
125	Crystallization and Organic Fieldâ€Effect Transistor Performance of a Hydrogenâ€Bonded Quaterthiophene. Chemistry - A European Journal, 2020, 26, 10265-10275.	1.7	5
126	Structureâ€“Property Relationships in Bithiophenes with Hydrogenâ€Bonded Substituents. Chemistry - A European Journal, 2021, 27, 3348-3360.	1.7	5

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127	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
128	Mapping Active Site Geometry to Activity in Immobilized Frustrated Lewis Pair Catalysts. Angewandte Chemie - International Edition, 2022, 61, .	7.2	5
129	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4
130	Can five-membered Te2N2S rings be considered aromatic?. Structural Chemistry, 2007, 18, 841-847.	1.0	3
131	Impact of quantum-chemical metrics on the machine learning prediction of electron density. Journal of Chemical Physics, 2021, 155, 024107.	1.2	3
132	Uncovering the Activity of Alkaline Earth Metal Hydrogenation Catalysis Through Molecular Volcano Plots. Topics in Catalysis, 2022, 65, 289-295.	1.3	3
133	Mapping Active Site Geometry to Activity in Immobilized Frustrated Lewis Pair Catalysts. Angewandte Chemie, 0, , .	1.6	3
134	Harvesting the fragment-based nature of bifunctional organocatalysts to enhance their activity. Organic Chemistry Frontiers, 2022, 9, 4041-4051.	2.3	3
135	How Robust Is the Reversible Steric Shielding Strategy for Photoswitchable Organocatalysts?. Journal of Organic Chemistry, 2022, 87, 8849-8857.	1.7	3
136	FB-ECDA: Fragment-based Electronic Coupling Decomposition Analysis for Organic Amorphous Semiconductors. Journal of Physical Chemistry A, 2020, 124, 10624-10634.	1.1	2
137	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
138	Methoxycyclization of 1,5â€Enynes by Coinage Metal Catalysts: Is Gold Always Superior?. Helvetica Chimica Acta, 2021, 104, e2100134.	1.0	2
139	Mapping Catalystâ€Solvent Interplay in Competing Carboamination/Cyclopropanation Reactions. Chemistry - A European Journal, 2022, , .	1.7	1