

Charles Edwin Webster

List of Publications by Year in descending order

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104
papers

3,858
citations

117453

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138251

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109
all docs

109
docs citations

109
times ranked

4264
citing authors

#	ARTICLE	IF	CITATIONS
1	Sensitized and Self-Sensitized Photocatalytic Carbon Dioxide Reduction Under Visible Light with Ruthenium Catalysts Shows Enhancements with More Conjugated Pincer Ligands. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	1.0	5
2	Triphenylene containing blue-light emitting semi-fluorinated aryl ether polymers with excellent thermal and photostability. <i>Materials Chemistry Frontiers</i> , 2022, 6, 1391-1404.	3.2	3
3	Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N ₂ O by Ru Pincer Complexes. <i>Inorganics</i> , 2022, 10, 69.	1.2	5
4	Low-Valent Cobalt(I) CNC Pincer Complexes as Catalysts for Light-Driven Carbon Dioxide Reduction. <i>ACS Catalysis</i> , 2022, 12, 8718-8728.	5.5	8
5	Predicting Absorption and Emission Maxima of Polycyclic Aromatic Azaborines: Reliable Transition Energies and Character. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3-12.	1.1	1
6	Singlet Oxygen Formation vs Photodissociation for Light-Responsive Protic Ruthenium Anticancer Compounds: The Oxygenated Substituent Determines Which Pathway Dominates. <i>Inorganic Chemistry</i> , 2021, 60, 2138-2148.	1.9	20
7	Benchmarking the Fluxional Processes of Organometallic Piano-Stool Complexes. <i>Molecules</i> , 2021, 26, 2310.	1.7	3
8	Light-Responsive and Protic Ruthenium Compounds Bearing Bathophenanthroline and Dihydroxybipyridine Ligands Achieve Nanomolar Toxicity towards Breast Cancer Cells. <i>Photochemistry and Photobiology</i> , 2021, , .	1.3	6
9	The curious case of DMSO: A CCSD(T)/CBS(aQ56+d) benchmark and DFT study. <i>Journal of Chemical Physics</i> , 2021, 155, 114304.	1.2	2
10	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. <i>Biophysical Journal</i> , 2021, 120, 3577-3587.	0.2	7
11	Structure-Functional Analysis of Hydrogen Production Catalyzed by Molecular Cobalt Complexes with Pentadentate Ligands in Aqueous Solutions. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3534-3547.	1.0	9
12	Tris(carbene) Stabilization of Monomeric Magnesium Cations: A Neutral, Nontethered Ligand Approach. <i>Organometallics</i> , 2020, 39, 4329-4339.	1.1	12
13	Planar, Stair-Stepped, and Twisted: Modulating Structure and Photophysics in Pyrene- and Benzene-Fused N-Heterocyclic Boranes. <i>Chemistry - A European Journal</i> , 2020, 26, 10072-10082.	1.7	6
14	Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO ₂ to CO with Ruthenium CNC Pincer Complexes. <i>ChemCatChem</i> , 2020, 12, 4879-4885.	1.8	7
15	Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2709-2717.	1.0	10
16	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. <i>Angewandte Chemie</i> , 2020, 132, 12794-12797.	1.6	3
17	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12694-12697.	7.2	25
18	Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents. <i>Organometallics</i> , 2019, 38, 688-696.	1.1	24

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19	Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction. <i>Inorganic Chemistry</i> , 2019, 58, 8012-8020.	1.9	49
20	Catalytic H ₂ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2134-2139.	1.0	14
21	Photocatalytic H ₂ -Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 16458-16474.	1.9	11
22	Extremely twisted and bent pyrene-fused N-heterocyclic germylenes. <i>Chemical Communications</i> , 2019, 55, 14954-14957.	2.2	5
23	The missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 128-135.	0.8	4
24	A Mononuclear Tungsten Photocatalyst for H ₂ Production. <i>ACS Catalysis</i> , 2018, 8, 4838-4847.	5.5	21
25	Nickel(η^5) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction. <i>Chemical Communications</i> , 2018, 54, 3819-3822.	2.2	39
26	Free methylidyne? CCC-NHC tantalum bis(imido) reactivity: protonation, rearrangement to a mixed unsymmetrical CCC-N-heterocyclic carbene/N-heterocyclic dicarbene (CCC-NHC/NHDC) pincer tantalum bis(imido) complex. <i>Inorganica Chimica Acta</i> , 2018, 469, 164-172.	1.2	10
27	Investigation of metallation/transmetallation reactions to synthesize a series of CCC-NHC Co pincer complexes and their X-ray structures. <i>Polyhedron</i> , 2018, 151, 568-574.	1.0	10
28	Computational Analysis of the Intramolecular Oxidative Amination of an Alkene Catalyzed by the Extreme η^5 -Loading N-Heterocyclic Carbene Pincer Tantalum(V) Bis(imido) Complex. <i>Organometallics</i> , 2018, 37, 1671-1681.	1.1	11
29	Electronic and Steric Tuning of Catalytic H ₂ Evolution by Cobalt Complexes with Pentadentate Polypyridyl-Amine Ligands. <i>Journal of the American Chemical Society</i> , 2018, 140, 9219-9229.	6.6	88
30	Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes. <i>Journal of the American Chemical Society</i> , 2018, 140, 9819-9822.	6.6	8
31	Synthesis of <i>C</i> -Unsubstituted 1,2-Diazetidines and Their Ring-Opening Reactions via Selective N-N Bond Cleavage. <i>Journal of Organic Chemistry</i> , 2018, 83, 9497-9503.	1.7	12
32	Iridium and Ruthenium Complexes of <i>N</i> -Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal. <i>Organometallics</i> , 2017, 36, 1091-1106.	1.1	94
33	Synthesis, characterization, photophysics, and a ligand rearrangement of CCC-NHC pincer nickel complexes: Colors, polymorphs, emission, and Raman spectra. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 258-265.	0.8	17
34	Phosphoramidate hydrolysis catalyzed by human histidine triad nucleotide binding protein 1 (hHint1): a cluster-model DFT computational study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8661-8668.	1.5	7
35	Electrocatalytic reduction of CO ₂ with CCC-NHC pincer nickel complexes. <i>Chemical Communications</i> , 2017, 53, 9442-9445.	2.2	53
36	Prediction of the reduction potential in transition-metal containing complexes: How expensive? For what accuracy?. <i>Journal of Computational Chemistry</i> , 2017, 38, 2430-2438.	1.5	23

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37	Synthesis, computational, and spectroscopic analysis of tunable highly fluorescent BN-1,2-azaborine derivatives containing the N-BOH moiety. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 10172-10183.	1.5	9
38	Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9982-9997.	1.1	6
39	Experimental and Computational Studies of the Mechanisms of Hydroamination/Cyclisation of Unactivated β,γ -Amino-alkenes with CCC-NHC Pincer Zr Complexes. <i>Australian Journal of Chemistry</i> , 2016, 69, 573.	0.5	10
40	The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores. <i>Journal of Organic Chemistry</i> , 2016, 81, 10955-10963.	1.7	17
41	Extreme π -Loading as a Design Element for Accessing Imido Ligand Reactivity. A CCC-NHC Pincer Tantalum Bis(imido) Complex: Synthesis, Characterization, and Catalytic Oxidative Amination of Alkenes. <i>Organometallics</i> , 2016, 35, 3452-3460.	1.1	31
42	Transmetallation from CCC-NHC pincer Zr complexes in the synthesis of air-stable CCC-NHC pincer Co(π) complexes and initial hydroboration trials. <i>Dalton Transactions</i> , 2016, 45, 2823-2828.	1.6	68
43	π -Boration of β,γ -unsaturated carbonyl compounds in ethanol and methanol catalyzed by CCC-NHC pincer Rh complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 802, 32-38.	0.8	27
44	The trans \rightarrow cis isomerization of Ni(β -2-TEMPO) ₂ : Interconnections and conformational complexity. <i>Inorganica Chimica Acta</i> , 2015, 436, 220-229.	1.2	2
45	A Theoretical Study of Phosphoryl Transfers of Tyrosyl-DNA Phosphodiesterase I (Tdp1) and the Possibility of a α -Dead-End-Phosphohistidine Intermediate. <i>Biochemistry</i> , 2015, 54, 4236-4247.	1.2	20
46	Synthesis, characterization, photophysical properties, and catalytic activity of an SCS bis(N-heterocyclic thione) (SCS-NHT) Pd pincer complex. <i>Dalton Transactions</i> , 2015, 44, 14475-14482.	1.6	41
47	Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 715-721.	1.0	9
48	Degenerate Pathways for Metallacycle Ring Inversions: A Common Phenomenon Consistent with the Principle of Microscopic Reversibility. <i>Organometallics</i> , 2014, 33, 5928-5931.	1.1	10
49	Theoretical studies of cyclic adenosine monophosphate dependent protein kinase: native enzyme and ground-state and transition-state analogues. <i>Dalton Transactions</i> , 2014, 43, 3039-3043.	1.6	5
50	Synthesis, Characterization, and X-ray Molecular Structure of Tantalum CCC-N-Heterocyclic Carbene (CCC-NHC) Pincer Complexes with Imidazole- and Triazole-Based Ligands. <i>Organometallics</i> , 2014, 33, 952-958.	1.1	30
51	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic H ₂ Evolution. <i>Inorganic Chemistry</i> , 2014, 53, 10094-10100.	1.9	79
52	<i>Organometallics</i> Roundtable 2013 \rightarrow 2014. <i>Organometallics</i> , 2014, 33, 1505-1527.	1.1	24
53	Photochemistry of Chromium Arene Tricarbonyl Complexes with Tethered Pyridinyl and Propenyl Groups: Investigations of the Effect of Ring Size on Chelate Formation, Structure, and Linkage Isomerization. <i>Organometallics</i> , 2014, 33, 485-497.	1.1	14
54	Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 13764-13774.	6.6	26

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55	Metal-Ligand Synergistic Effects in the Complex Ni(η^2 -TEMPO) $_2$: Synthesis, Structures, and Reactivity. <i>Inorganic Chemistry</i> , 2013, 52, 13882-13893.	1.9	13
56	Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter. <i>Dalton Transactions</i> , 2013, 42, 8820.	1.6	33
57	Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15792-15803.	1.2	19
58	Near attack conformers dominate η^2 -phosphoglucomutase complexes where geometry and charge distribution reflect those of substrate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 6910-6915.	3.3	47
59	Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7261-7271.	1.1	36
60	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. <i>Organometallics</i> , 2012, 31, 1664-1672.	1.1	104
61	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. <i>Organometallics</i> , 2012, 31, 4055-4062.	1.1	19
62	Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5941-5944.	7.2	280
63	Engineering Femtosecond Organometallic Chemistry: Photochemistry and Dynamics of Ultrafast Chelation of Cyclopentadienylmanganese Tricarbonyl Derivatives with Pendant Benzenecarbonyl and Pyridinecarbonyl Groups. <i>Organometallics</i> , 2011, 30, 5611-5619.	1.1	26
64	Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands. <i>Inorganic Chemistry</i> , 2011, 50, 10564-10571.	1.9	80
65	Ligand Displacement from $\text{TpMn}(\text{CO})_2\text{L}$ Complexes: A Large Rate Enhancement in Comparison to the $\text{CpMn}(\text{CO})_2\text{L}$ Analogues. <i>Organometallics</i> , 2011, 30, 3054-3063.	1.1	13
66	Bond Energies, Reaction Volumes, and Kinetics for η^5 - and η^6 -Complexes of $\text{Mo}(\text{CO})_5\text{L}$. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9004-9013.	1.1	6
67	Time-resolved IR Studies on the Mechanism for the Functionalization of Primary C-H Bonds by Photoactivated $\text{Cp}^*\text{W}(\text{CO})_3(\text{Bpin})$. <i>Journal of the American Chemical Society</i> , 2010, 132, 1848-1859.	6.6	41
68	Development of Ultrafast Photochromic Organometallics and Photoinduced Linkage Isomerization of Arene Chromium Carbonyl Derivatives. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2666-2676.	1.1	48
69	Theoretical study of the biologically important dioxo diiron diamond core structures. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 467-478.	0.5	2
70	Disulfido iron-manganese carbonyl cluster complexes: Synthesis, structure, bonding and properties of the radical $\text{CpFeMn}_2(\text{CO})_7(\mu_3\text{-S})_2$. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 2732-2738.	0.8	10
71	Linkage Isomerization as a Mechanism for Photochromic Materials: Cyclopentadienylmanganese Tricarbonyl Derivatives with Chelatable Functional Groups. <i>Organometallics</i> , 2008, 27, 289-296.	1.1	52
72	Probing the Mechanism of Carbon-Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. <i>Organometallics</i> , 2008, 27, 189-201.	1.1	29

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73	Carbon-Hydrogen Bond Activation in Hydridotrtris(pyrazolyl)borate Platinum(IV) Complexes: Comparison of Density Functionals, Basis Sets, and Bonding Patterns. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2268-2281.	2.3	14
74	Computational Insights into Degenerate Ethylene Exchange with a Grubbs-Type Catalyst. <i>Journal of the American Chemical Society</i> , 2007, 129, 7490-7491.	6.6	44
75	Forty years of Fenske-Hall molecular orbital theory. , 2005, , 1143-1165.		13
76	Electronic and Steric Effects on Molecular Dihydrogen Activation in $[\text{Cp}^*\text{OsH}_4(\text{L})]^+(\text{L} = \text{PPh}_3, \text{AsPh}_3)$. <i>Journal of the American Chemical Society</i> , 2005, 127, 1070-1077.	6.6	33
77	Urea decomposition facilitated by a urease model complex: a theoretical investigation. <i>Dalton Transactions</i> , 2005, , 3542.	1.6	17
78	Rhodium Boryl Complexes in the Catalytic, Terminal Functionalization of Alkanes. <i>Journal of the American Chemical Society</i> , 2005, 127, 2538-2552.	6.6	317
79	High Nuclearity Iridium-Platinum Clusters: Synthesis, Structures, Bonding, and Reactivity. <i>Journal of the American Chemical Society</i> , 2005, 127, 1007-1014.	6.6	34
80	Rhodium Silyl Boryl Hydride Complexes: Comparison of Bonding and the Rates of Elimination of Borane, Silane, and Dihydrogen. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5474-5477.	7.2	41
81	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. <i>Inorganic Chemistry</i> , 2004, 43, 4127-4136.	1.9	58
82	Structures and Energetics of Models for the Active Site of Acetyl-Coenzyme A Synthase: Role of Distal and Proximal Metals in Catalysis. <i>Journal of the American Chemical Society</i> , 2004, 126, 3410-3411.	6.6	59
83	Reaction of the 1,8-Bis(diphenylmethyl)naphthalenediyl Dication with Fluoride: Formation of a Cation Containing a C-F-C Bridge. <i>Journal of the American Chemical Society</i> , 2004, 126, 8189-8196.	6.6	43
84	Dinuclear Ruthenium and Iron Complexes Containing Palladium and Platinum with Tri-tert-Butylphosphine Ligands: Synthesis, Structures, and Bonding. <i>Inorganic Chemistry</i> , 2004, 43, 3921-3929.	1.9	30
85	Superloading of Tin Ligands into Rhodium and Iridium Carbonyl Cluster Complexes. <i>Inorganic Chemistry</i> , 2004, 43, 7576-7578.	1.9	66
86	Bimetallic Cluster Complexes: The Synthesis, Structures, and Bonding of Ruthenium Carbonyl Cluster Complexes Containing Palladium and Platinum with the Bulky Tri-tert-butyl-phosphine Ligand. <i>Journal of the American Chemical Society</i> , 2004, 126, 5253-5267.	6.6	64
87	Nickel-Manganese Sulfido Carbonyl Cluster Complexes. Synthesis, Structure, and Properties of the Unusual Paramagnetic Complexes $\text{Cp}_2\text{Ni}_2\text{Mn}(\text{CO})_3(\eta^3\text{-E})_2$, E = S, Se. <i>Inorganic Chemistry</i> , 2004, 43, 2515-2525.	1.9	32
88	High-Energy Intermediate or Stable Transition State Analogue: Theoretical Perspective of the Active Site and Mechanism of β -Phosphoglucomutase. <i>Journal of the American Chemical Society</i> , 2004, 126, 6840-6841.	6.6	41
89	De Novo design in organometallic chemistry: stabilizing iridium(V). <i>Coordination Chemistry Reviews</i> , 2003, 238-239, 315-331.	9.5	28
90	Experimental and Computational Evidence for a Boron-Assisted, β -Bond Metathesis Pathway for Alkane Borylation. <i>Journal of the American Chemical Society</i> , 2003, 125, 858-859.	6.6	177

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91	The role of triplet states in the long wavelength absorption region of bromine nitrate. <i>Journal of Chemical Physics</i> , 2003, 119, 7864-7870.	1.2	5
92	Factors affecting the structure of substituted tris(pyrazolyl)borate rhodium dicarbonyl complexes. <i>Inorganica Chimica Acta</i> , 2002, 330, 268-282.	1.2	21
93	The vibrational spectrum of Tp3,5-MeRhH2(H2): a computational and inelastic neutron scattering study. <i>Inorganica Chimica Acta</i> , 2002, 330, 240-249.	1.2	9
94	The Theoretical Transition State Structure of a Model Complex Bears a Striking Resemblance to the Active Site Structure of DMSO Reductase. <i>Journal of the American Chemical Society</i> , 2001, 123, 5820-5821.	6.6	81
95	Minimum Energy Structure of Hydridotris(pyrazolyl)borato Iridium(V) Tetrahydride Is Not a C _{3v} Capped Octahedron. <i>Journal of the American Chemical Society</i> , 2001, 123, 9822-9829.	6.6	20
96	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 20. Carbon-Hydrogen and Carbon-Carbon Bond Activation of Cyclopropane by Cationic Iridium(III) and Neutral Rhodium(I) and Iridium(I) Complexes. <i>Organometallics</i> , 2001, 20, 5606-5613.	1.1	27
97	A thermodynamic analysis of the Calad method with respect to gas-solid calorimetry. <i>Microporous and Mesoporous Materials</i> , 1999, 31, 205-209.	2.2	5
98	The multiple equilibrium analysis quantitative prediction of single and multi-component adsorption isotherms on carbonaceous and zeolitic solids. <i>Microporous and Mesoporous Materials</i> , 1999, 33, 291-306.	2.2	19
99	Extension of the electrostatic-covalent model to 2:1 adducts. <i>Polyhedron</i> , 1999, 18, 1097-1106.	1.0	4
100	Multiple Equilibrium Analysis Description of Adsorption on Na-Mordenite and H-Mordenite. <i>Journal of the American Chemical Society</i> , 1999, 121, 12127-12139.	6.6	59
101	A Method for Characterizing Effective Pore Sizes of Catalysts. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1242-1249.	1.2	65
102	Exploring Surfaces and Cavities in Lipoxygenase and Other Proteins by Hyperpolarized Xenon-129 NMR. <i>Journal of the American Chemical Society</i> , 1999, 121, 9370-9377.	6.6	54
103	A Multiple-Process Equilibrium Analysis of Silica Gel and HZSM-5. <i>Journal of the American Chemical Society</i> , 1998, 120, 538-547.	6.6	37
104	Molecular Dimensions for Adsorptives. <i>Journal of the American Chemical Society</i> , 1998, 120, 5509-5516.	6.6	353