

Jorge J CarbÃ³

List of Publications by Year in descending order

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papers

4,643
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81839

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times ranked

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#	ARTICLE	IF	CITATIONS
1	Nâ•N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. <i>Inorganic Chemistry</i> , 2022, 61, 474-485.	1.9	5
2	Computational Modelling of the Interactions Between Polyoxometalates and Biological Systems. <i>Frontiers in Chemistry</i> , 2022, 10, 876630.	1.8	9
3	Effective Storage of Electrons in Water by the Formation of Highly Reduced Polyoxometalate Clusters. <i>Journal of the American Chemical Society</i> , 2022, 144, 8951-8960.	6.6	37
4	Reaction Pathway Discrimination in Alkene Oxidation Reactions by Designed Tiâ€Siolyâ€Polyoxometalates. <i>ChemCatChem</i> , 2021, 13, 1220-1229.	1.8	13
5	Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. <i>Inorganic Chemistry</i> , 2021, 60, 807-815.	1.9	5
6	Mapping the Electronic Structure and the Reactivity Trends for Stabilized Î±â€Boryl Carbanions. <i>Chemistry - A European Journal</i> , 2021, 27, 12352-12361.	1.7	10
7	Activation of H ₂ O ₂ over Zr(IV). Insights from Model Studies on Zr-Monosubstituted Lindqvist Tungstates. <i>ACS Catalysis</i> , 2021, 11, 10589-10603.	5.5	25
8	Alkoxide activation of tetra-alkoxy diboron reagents in Câ€B bond formation: a decade of unpredictable reactivity. <i>Chemical Communications</i> , 2021, 57, 11935-11947.	2.2	20
9	Transborylation of alkenylboranes with diboranes. <i>Chemical Communications</i> , 2021, 57, 13361-13364.	2.2	13
10	Regioselectivity Control in Pd-Catalyzed Telomerization of Isoprene Enabled by Solvent and Ligand Selection. <i>ACS Catalysis</i> , 2020, 10, 11458-11465.	5.5	9
11	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. <i>ACS Catalysis</i> , 2020, 10, 13455-13467.	5.5	13
12	Frontispiece: Structureâ€Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. <i>Chemistry - A European Journal</i> , 2020, 26, .	1.7	0
13	Structureâ€Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. <i>Chemistry - A European Journal</i> , 2020, 26, 5799-5809.	1.7	31
14	Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. <i>ACS Catalysis</i> , 2020, 10, 4737-4750.	5.5	45
15	Consecutive borylcupration/Câ€C coupling of Î³-alkenyl aldehydes towards diastereoselective 2-(borylmethyl)cycloalkanols. <i>Chemical Communications</i> , 2020, 56, 5973-5976.	2.2	11
16	2 Mechanistic Aspects of Carbonâ€Boron Bond Formation. , 2020, , .		0
17	9-Cobalt(II)-Containing 27-Tungsto-3-germanate(IV): Synthesis, Structure, Computational Modeling, and Heterogeneous Water Oxidation Catalysis. <i>Inorganic Chemistry</i> , 2019, 58, 11308-11316.	1.9	23
18	A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. <i>Inorganic Chemistry</i> , 2019, 58, 12157-12166.	1.9	4

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19	Why Does Nb(V) Show Higher Heterolytic Pathway Selectivity Than Ti(IV) in Epoxidation with H ₂ O ₂ ? Answers from Model Studies on Nb- and Ti-Substituted Lindqvist Tungstates. <i>ACS Catalysis</i> , 2019, 9, 6262-6275.	5.5	36
20	How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with [V ₁₈ O ₄₂] ^{q-} (q = 3, 5, 7, 11, and 13). <i>Inorganic Chemistry</i> , 2019, 58, 3881-3894.	1.9	18
21	Transition-Metal-Free Allylic Borylation of 1,3-Dienes. <i>Organic Letters</i> , 2019, 21, 2251-2255.	2.4	21
22	Copper-Catalyzed Borylative Ring Closing C-C Coupling toward Spiro- and Dispiroheterocycles. <i>ACS Catalysis</i> , 2018, 8, 2833-2838.	5.5	40
23	Self-assembly study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach. <i>Dalton Transactions</i> , 2018, 47, 6304-6313.	1.6	30
24	Polyoxometalate electrocatalysts based on earth-abundant metals for efficient water oxidation in acidic media. <i>Nature Chemistry</i> , 2018, 10, 24-30.	6.6	375
25	Modeling the Oxygen Vacancy at a Molecular Vanadium(III) Silica-Supported Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 14903-14914.	6.6	26
26	Relevance of Protons in Heterolytic Activation of H ₂ O ₂ over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. <i>ACS Catalysis</i> , 2018, 8, 9722-9737.	5.5	52
27	Understanding the mechanism of transition metal-free <i>anti</i> addition to alkynes: the selenoboration case. <i>Catalysis Science and Technology</i> , 2018, 8, 3617-3628.	2.1	13
28	Transition-Metal-Free Stereoselective Borylation of Allenamides. <i>Chemistry - A European Journal</i> , 2018, 24, 14059-14063.	1.7	18
29	Quantitative Structure-Activity Relationships for the Nucleophilicity of Trivalent Boron Compounds. <i>Chemistry - A European Journal</i> , 2017, 23, 5066-5075.	1.7	15
30	Core-substituted naphthalenediimides anchored on BiVO ₄ for visible light-driven water splitting. <i>Green Chemistry</i> , 2017, 19, 2448-2462.	4.6	11
31	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. <i>Journal of Catalysis</i> , 2017, 350, 56-63.	3.1	59
32	[Co ₉ (H ₂ O) ₆ (OH) ₃ (HPO ₄) ₂ (PW ₉ O ₃₄) ₃] ¹⁶⁻ . <i>Advances in Inorganic Chemistry</i> , 2017, , 155-179.	0.4	2
33	Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. <i>Inorganic Chemistry</i> , 2017, 56, 4148-4156.	1.9	15
34	Size and charge effect of guest cations in the formation of polyoxopalladates: a theoretical and experimental study. <i>Chemical Science</i> , 2017, 8, 7862-7872.	3.7	20
35	Intermetallic Cooperation in C-H Activation Involving Transient Titanium-Alkylidene Species: A Synthetic and Mechanistic Study. <i>Organometallics</i> , 2017, 36, 3076-3083.	1.1	14
36	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted β -Keggin Polyoxotungstate. <i>ACS Catalysis</i> , 2017, 7, 8514-8523.	5.5	23

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37	Real-time molecular scale observation of crystal formation. <i>Nature Chemistry</i> , 2017, 9, 369-373.	6.6	69
38	Diskrete Silber(I)â€Palladium(II)â€Oxoâ€Nanocluster, {Ag ₄ Pd ₁₃ } und {Ag ₅ Pd ₁₅ }, sowie die Rolle der Metallâ€Metallâ€Bindung induziert durch Kationenâ€Einschluss. <i>Angewandte Chemie</i> , 2016, 128, 15998-16002.	1.6	7
39	Discrete Silver(I)â€Palladium(II)â€Oxo Nanoclusters, {Ag ₄ Pd ₁₃ } and {Ag ₅ Pd ₁₅ }, and the Role of Metalâ€Metal Bonding Induced by Cation Confinement. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15766-15770.	7.2	31
40	Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented Î ² -Oxygen Transfer Mechanism. <i>Inorganic Chemistry</i> , 2016, 55, 6080-6084.	1.9	40
41	Arene C(sp ²)-H Metalation at Ni ^{II} Modeled with a Reactive PONC _{Ph} Ligand. <i>Inorganic Chemistry</i> , 2016, 55, 8041-8047.	1.9	32
42	Photoreduction Mechanism of CO ₂ to CO Catalyzed by a Rhenium(I)â€Polyoxometalate Hybrid Compound. <i>ACS Catalysis</i> , 2016, 6, 6422-6428.	5.5	58
43	Probing Polyoxometalateâ€Protein Interactions Using Molecular Dynamics Simulations. <i>Chemistry - A European Journal</i> , 2016, 22, 15280-15289.	1.7	50
44	Mechanism of Thioether Oxidation over Diâ€and Tetrameric Ti Centres: Kinetic and DFT Studies Based on Model Tiâ€Containing Polyoxometalates. <i>Chemistry - A European Journal</i> , 2015, 21, 14496-14506.	1.7	27
45	Selective Carbonâ€Carbon Bond Activation of Oxirane by a Bisphosphine Pt(0) Complexâ€A Theoretical Study. <i>Organometallics</i> , 2015, 34, 3764-3773.	1.1	3
46	Mixed diboration of alkenes in a metal-free context. <i>Chemical Communications</i> , 2015, 51, 1693-1696.	2.2	77
47	Carbonâ€Nitrogen Bond Construction and Carbonâ€Oxygen Double Bond Cleavage on a Molecular Titanium Oxonitride: A Combined Experimental and Computational Study. <i>Inorganic Chemistry</i> , 2015, 54, 9401-9412.	1.9	12
48	Unsymmetrical 1,1-diborated multisubstituted sp ³ -carbons formed via a metal-free concerted-asynchronous mechanism. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 9659-9664.	1.5	66
49	A fast metalâ€metal bonded water oxidation catalyst. <i>Journal of Catalysis</i> , 2014, 315, 25-32.	3.1	20
50	A theoretical study of the activity in Rh-catalysed hydroformylation: the origin of the enhanced activity of the Î-acceptor phosphinine ligand. <i>Catalysis Science and Technology</i> , 2014, 4, 979-987.	2.1	30
51	Alkaline Earth Guests in Polyoxopalladate Chemistry: From Nanocube to Nanostar via an Openâ€Shell Structure. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11974-11978.	7.2	59
52	Aerobic Carbonâ€Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide. <i>Journal of the American Chemical Society</i> , 2014, 136, 10941-10948.	6.6	77
53	Pdâ€Catalysed Monoâ€and Dicarboxylation of Aryl Iodides: Insights into the Mechanism and the Selectivity. <i>Chemistry - A European Journal</i> , 2014, 20, 10982-10989.	1.7	26
54	A Clearâ€Cut Example of Selective Bpinî;Bdan Activation and Precise Bdan Transfer on Boron Conjugate Addition. <i>Chemistry - A European Journal</i> , 2014, 20, 3616-3620.	1.7	59

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55	Nature of Zr-Monosubstituted Monomeric and Dimeric Polyoxometalates in Water Solution at Different pH Conditions: Static Density Functional Theory Calculations and Dynamic Simulations. <i>Inorganic Chemistry</i> , 2014, 53, 778-786.	1.9	22
56	Understanding $\hat{1},\hat{1}^2$ -Unsaturated Imine Formation from Amine Additions to $\hat{1},\hat{1}^2$ -Unsaturated Aldehydes and Ketones: An Analytical and Theoretical Investigation. <i>Journal of Organic Chemistry</i> , 2014, 79, 5163-5172.	1.7	43
57	Structure and Reactivity of Polyoxometalates. , 2013, , 887-906.		2
58	Cobalt Polyoxometalates as Heterogeneous Water Oxidation Catalysts. <i>Inorganic Chemistry</i> , 2013, 52, 4753-4755.	1.9	118
59	Redox-Active Behavior of the $[\{Ti(\hat{1}^5-C\hat{5}Me\hat{5})(\hat{1}^4-NH)\}_3(\hat{1}^4-N)]$ Metalloligand. <i>Inorganic Chemistry</i> , 2013, 52, 6103-6109.	1.9	8
60	Polyoxopalladates Encapsulating 8-Coordinated Metal Ions, $[MO_8Pd_{12}L_8]^{n-}$ ($M = Ti, Zr, Hf$)	1.9	58
61	13214-13228. Structure, properties and reactivity of polyoxometalates: a theoretical perspective. <i>Chemical Society Reviews</i> , 2012, 41, 7537.	18.7	392
62	Disclosing the Structure/Activity Correlation in Trivalent Boron-Containing Compounds: A Tendency Map. <i>Chemistry - A European Journal</i> , 2012, 18, 12794-12802.	1.7	69
63	Predicting the Enantioselectivity of the Copper-Catalysed Cyclopropanation of Alkenes by Using Quantitative Quadrant-Diagram Representations of the Catalysts. <i>Chemistry - A European Journal</i> , 2012, 18, 14026-14036.	1.7	39
64	Alkene oxidation by Ti-containing polyoxometalates. Unambiguous characterization of the role of the protonation state. <i>Chemical Communications</i> , 2012, 48, 9266.	2.2	48
65	3D-QSPR models for predicting the enantioselectivity and the activity for asymmetric hydroformylation of styrene catalyzed by Rh-diphosphane. <i>Catalysis Science and Technology</i> , 2012, 2, 1694.	2.1	35
66	Trivalent boron nucleophile as a new tool in organic synthesis: reactivity and asymmetric induction. <i>Chemical Society Reviews</i> , 2012, 41, 3558.	18.7	220
67	Theoretical Studies of Asymmetric Hydroformylation Using the Rh-BINAPHOS Catalyst: Origin of Coordination Preferences and Stereinduction. <i>Chemistry - A European Journal</i> , 2012, 18, 995-1005.	1.7	45
68	Catalytic Non-Conventional <i>trans</i> -Hydroboration: A Theoretical and Experimental Perspective. <i>Chemistry - A European Journal</i> , 2012, 18, 1512-1521.	1.7	54
69	Ammonia Activation by $\hat{1}^3$ -Alkyldiyne Fragments Supported on a Titanium Molecular Oxide Model. <i>Inorganic Chemistry</i> , 2011, 50, 6269-6279.	1.9	39
70	Theoretical characterization of a Ru N-Heterocyclic Carbene derivative of a polyoxometalate. Enhanced π -interaction in oxide supported TM-organic linkages. <i>Dalton Transactions</i> , 2011, 40, 2975.	1.6	8
71	Discovering the chemical reactivity of the molecular oxonitride $[\{Ti(\hat{1}^5-C_5Me_5)(\hat{1}^4-O)\}_3(\hat{1}^4-N)]$. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 4011-4017.	0.8	9
72	Current trends in the computational modelling of polyoxometalates. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 393-404.	0.5	69

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73	Epoxidation of Alkenes with H ₂ O ₂ Catalyzed by Ditungsten-Containing Tungstodisarsenate(III): Experimental and Theoretical Studies. <i>European Journal of Inorganic Chemistry</i> , 2010, 2010, 5312-5317.	1.0	42
74	Polyoxopalladates Encapsulating Yttrium and Lanthanide Ions, [X ^{III} Pd ^{II}] ₁₂ (AsPh) ₈ O ₃₂ ·5H ₂ O (X=Y, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu). <i>Chemistry - A European Journal</i> , 2010, 16, 9076-9085.	1.7	81
75	Mechanistic Insights into Alkene Epoxidation with H ₂ O ₂ by Ti- and other TM-Containing Polyoxometalates: Role of the Metal Nature and Coordination Environment. <i>Journal of the American Chemical Society</i> , 2010, 132, 7488-7497.	6.6	148
76	Lewis Base Behavior of Bridging Nitrido Ligands of Titanium Polynuclear Complexes. <i>Chemistry - A European Journal</i> , 2009, 15, 11619-11631.	1.7	13
77	Hydrogen-Transfer Processes Involving an Organotitanium Oxide and Alcohols. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 643-653.	1.0	13
78	Experimental and Computational Study of the Bonding Properties of Mixed Bisphosphido Ylides of Phosphorus and Sulfur. <i>Inorganic Chemistry</i> , 2009, 48, 6823-6834.	1.9	16
79	Quantifying the Donor-Acceptor Properties of Phosphine and N-Heterocyclic Carbene Ligands in Grubbs' Catalysts Using a Modified EDA Procedure Based on Orbital Deletion. <i>Organometallics</i> , 2009, 28, 4283-4287.	1.1	57
80	The Rate-Determining Step in the Rhodium-Xantphos-Catalysed Hydroformylation of 1-Octene. <i>Chemistry - A European Journal</i> , 2008, 14, 1843-1853.	1.7	75
81	Construction of Titanasiloxanes by Incorporation of Silanols to the Metal Oxide Model [Ti ^V OC ₅ Me ₅] ₃ (¹ / ₄ Cr): DFT Elucidation of the Reaction Mechanism. <i>Chemistry - A European Journal</i> , 2008, 14, 7930-7938.	2.0	20
82	On the Origin of Alternating Bond Distortions and the Emergence of Chirality in Polyoxometalate Anions. <i>Journal of the American Chemical Society</i> , 2008, 130, 8223-8233.	6.6	107
83	Influence of polyoxometalate ligands on the nature of high-valent transition metal nitrido species. A theoretical analysis of experimentally known and unprecedented compounds. <i>Dalton Transactions</i> , 2008, , 5166.	1.6	38
84	Influence of the Nature of the Ligand on Dirhodium(II) Carbene Species: A Theoretical Analysis. <i>Organometallics</i> , 2008, 27, 2873-2876.	1.1	22
85	¹ H NMR Investigation of Paramagnetic Chromium(III) Olefin Polymerization Catalysts: Experimental Results, Shift Assignment and Prediction by Quantum Chemical Calculations. <i>Organometallics</i> , 2007, 26, 4402-4412.	1.1	80
86	Palladium-NHC complexes do catalyse the diboration of alkenes: mechanistic insights. <i>Chemical Communications</i> , 2007, , 3380.	2.2	59
87	New Quantum Mechanics-Based Three-Dimensional Molecular Descriptors for Use in QSSR Approaches: Application to Asymmetric Catalysis. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2228-2234.	2.5	48
88	Electronic Ligand Effects on the Regioselectivity of the Rhodium-Diphosphine-Catalyzed Hydroformylation of Propene. <i>Organometallics</i> , 2007, 26, 2234-2242.	1.1	30
89	Addition of Terminal Alkynes to a Molecular Titanium-Zinc Nitride. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 3095-3098.	7.2	20
90	ZrIV-Monosubstituted Keggin-Type Dimeric Polyoxometalates: Synthesis, Characterization, Catalysis of H ₂ O ₂ -Based Oxidations, and Theoretical Study. <i>Inorganic Chemistry</i> , 2006, 45, 7224-7234.	1.9	113

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91	Mixed P ⁺ N and As ⁺ N Bis-Ylide Palladium Complexes: Cooperative Intramolecular Interactions, Conformational Preferences, and C-H Bond Activations. <i>Organometallics</i> , 2006, 25, 4653-4664.	1.1	31
92	Palladium Complexes of a Phosphorus Ylide with Two Stabilizing Groups: Synthesis, Structure, and DFT Study of the Bonding Modes. <i>Inorganic Chemistry</i> , 2006, 45, 6803-6815.	1.9	49
93	Origin of Stereinduction by Chiral Aminophosphane Phosphinite Ligands in Enantioselective Catalysis: Asymmetric Hydroformylation. <i>Chemistry - A European Journal</i> , 2006, 12, 1457-1467.	1.7	36
94	Strong 1,4-P=O intramolecular interactions as a source of conformational preferences in $\hat{\pm}$ -stabilised phosphorus ylides. Part 2: metallic complexes. <i>Inorganica Chimica Acta</i> , 2004, 357, 1444-1456.	1.2	15
95	Synthesis and Characterization of PdII Complexes with Bis-Pyridinium and Isoquinolinium N-Ylides: Moderate CH ⁺ OC Intramolecular Hydrogen Bonds as Source of Conformational Preferences. <i>Inorganic Chemistry</i> , 2004, 43, 7622-7635.	1.9	15
96	Self-Consistency versus $\hat{\epsilon}$ Best-Fit Approaches in Understanding the Structure of Metal Nitrosyl Complexes. <i>Organometallics</i> , 2004, 23, 6008-6014.	1.1	5
97	Rhodium Diphosphine Hydroformylation. <i>ChemInform</i> , 2003, 34, no.	0.1	0
98	First X-ray Characterization and Theoretical Study of $\hat{\epsilon}$ -Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp* ⁺ Ru(PEt ₃) ₂] ⁺ . <i>Journal of the American Chemical Society</i> , 2003, 125, 3311-3321.	6.6	90
99	Two- and Four-Electron Alkyne Ligands in Osmium ⁺ Cyclopentadienyl Chemistry: Consequences of the $\hat{\epsilon}$ Interaction. <i>Organometallics</i> , 2002, 21, 305-314.	1.1	54
100	Rhodium Diphosphine Hydroformylation. <i>Catalysis By Metal Complexes</i> , 2002, , 161-187.	0.6	2
101	The reaction of the unsaturated rhenium fragment {Re($\hat{\epsilon}$ -C ₅ Me ₅)(CO) ₂ } with 1,4-difluorobenzene. Thermal intramolecular conversion of a rhenium (difluorophenyl)(hydride) to Re($\hat{\epsilon}$ -2-C ₆ H ₄ F ₂) and a [1,4]-metallotropic shift. <i>Dalton Transactions RSC</i> , 2001, , 1452-1461.	2.3	42
102	Unraveling the Origin of Regioselectivity in Rhodium Diphosphine Catalyzed Hydroformylation. A DFT QM/MM Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 7630-7637.	6.6	141
103	Strong 1,4-P=O Intramolecular Interactions as a Source of Conformational Preferences in $\hat{\pm}$ -Stabilized Phosphorus Ylides. <i>Inorganic Chemistry</i> , 2001, 40, 4913-4917.	1.9	32
104	Synthesis, molecular structure and computational study of a ruthenium bis(thietane) complex. <i>Inorganica Chimica Acta</i> , 2001, 316, 13-18.	1.2	5
105	Carbonylative Cycloaddition of Allyl Halides and Acetylenes Promoted by Ni(CO) ₄ . A DFT Study on the Reaction Mechanism. <i>Organometallics</i> , 2000, 19, 3516-3526.	1.1	10
106	Facile Synthesis of Alkynyl ⁺ and Vinylidene ⁺ Niobocene Complexes. Unexpected $\hat{\epsilon}$ -1-Vinylidene ⁺ $\hat{\epsilon}$ -2-Alkyne Isomerization. <i>Organometallics</i> , 2000, 19, 1749-1765.	1.1	32