Ab initio effective core potentials for molecular calculat transition metal atoms Sc to Hg

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Citation Report

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#	ARTICLE	IF	CITATIONS
3510	First-principles calculations of atomic and electronic structure of mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> <mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn (011)="" .<="" 2008,="" 77,="" and="" b,="" physical="" review="" surfaces.="" td=""><td>> 3 < /mml:1</td><td>nn></td></mml:mn></mml:msub></mml:mrow>	> 3 < /mml:1	nn>
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3562	Linkage Isomerization Reactions of M(CO)2L Complexes (M = (η5-C5H5)Mn, (η5-C5H5)Re, or (η6-C6H6)Cr; L =) Tj	ϳ <u>ξ</u> ΤΩq0 0	0 rgBT /Over
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	PONDX or palladates Encansulating X-Coordinated Metallions		
5023	[MO ₈ Pd ^{II} ₁₂ L ₈] ^{<i>n</i> i>â^'} (M =) Tj ETQq1 1 0	.784314 rş 1.9	gBT /Overloci 58
5023 5024	Polyoxopaliagates encapsulating 6-Coordinated Metallions,		
	[MO ₈ Pd ^{II} ₁₂ L ₈] ^{<i>n</i>i) a^'} (M =) Tj ETQq1 1 0 13214-13228. Mechanistic Features of Isomerizing Alkoxycarbonylation of Methyl Oleate. Journal of the American	1.9	58
5024	[MO ₈ Pd ^{II} ₁₂ L ₈] ^{(i>ni)<a^*< sup=""> (M =) Tj ETQq1 1 0 13214-13228. Mechanistic Features of Isomerizing Alkoxycarbonylation of Methyl Oleate. Journal of the American Chemical Society, 2012, 134, 17696-17703. An ab initio and DFT study of homolytic substitution reactions by oxyacyl radicals at sulfur, selenium,</a^*<>}	6.6	137
5024 5025	[MO⟨sub⟩8⟨/sub⟩Pd⟨sup⟩II⟨/sup⟩⟨sub⟩12⟨/sub⟩L⟨sub⟩8⟨/sub⟩]⟨sup⟩⟨i⟩n⟨/i⟩â°⟨/sup⟩ (M =) Tj ETQq1 1 0 13214-13228. Mechanistic Features of Isomerizing Alkoxycarbonylation of Methyl Oleate. Journal of the American Chemical Society, 2012, 134, 17696-17703. An ab initio and DFT study of homolytic substitution reactions by oxyacyl radicals at sulfur, selenium, and tellurium. Tetrahedron, 2012, 68, 10482-10488. The Reaction Mechanism of the Enantioselective Tsuji Allylation: Inner-Sphere and Outer-Sphere Pathways, Internal Rearrangements, and Asymmetric C–C Bond Formation. Journal of the American	1.9	58 137 6
5024 5025 5026	[MÓ ₈ Pd ^{II} ₁₂ L ₈] ^{<i>n</i> 10}	1.9 6.6 1.0 6.6	58 137 6 103
5024 5025 5026 5027	[MO ₈ Pd ^{II} ₁₂ L ₈] ^{<i>n</i>Pi ETQq1 1 0 1 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1}	1.9 6.6 1.0 6.6	58 137 6 103
5024 5025 5026 5027	[MO ₈ Pd ^{II} csub>12Ecsub>8] ^{ci>nparticles (M =) Tj ETQq1 10 13214-13228 Mechanistic Features of Isomerizing Alkoxycarbonylation of Methyl Oleate. Journal of the American Chemical Society, 2012, 134, 17696-17703. An ab initio and DFT study of homolytic substitution reactions by oxyacyl radicals at sulfur, selenium, and tellurium. Tetrahedron, 2012, 68, 10482-10488. The Reaction Mechanism of the Enantioselective Tsuji Allylation: Inner-Sphere and Outer-Sphere Pathways, Internal Rearrangements, and Asymmetric Câé"C Bond Formation. Journal of the American Chemical Society, 2012, 134, 19050-19060. An Efficient PIFA-Mediated Synthesis of a Directly Linked Zinc Chlorin Dimer via Regioselective Oxidative Coupling. Organic Letters, 2012, 14, 2746-2749. Highly Variable Zrâé"CH Highly Variable Zrâé"CH Highly Variable Zrâé"CH Ligand Coordination Modes. Organometallics, 2012, 31, 8208-8217. Cobalt Electrolyte/Dye Interactions in Dye-Sensitized Solar Cells: A Combined Computational and}	1.9 6.6 1.0 6.6 2.4	58 137 6 103 31 39

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6464	peroxotungstates ([SeO ₄ WO(O ₂) ₂ MO(O ₂) ₂) ₂) _{>2}) ₂) <s< td=""><td>sup>â^'<!--</td--><td>sup>) Tj</td></td></s<>	sup>â^' </td <td>sup>) Tj</td>	sup>) Tj
6465	Theoretical study on the electronic structures and optical properties of blue-green and blue phosphorescent iridium(III) complexes with tetraphenylimidodiphosphinate ligand. International Journal of Quantum Chemistry, 2014, 114, 183-191.	1.0	6
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9867	A half-sandwich Ta ^V dichlorido complex containing an <i>O</i> , <i>N</i> , <i>O</i> , Section C, Structural Chemistry, 2019, 75, 248-254.	0.2	4
9867 9868	<i>>O</i> , <i>N</i> , <i>Ö</i> ,i>′-tridentate Schiff base ligand: synthesis, crystal structure and <i>in</i>	1.0	4
	⟨i>O⟨ i>,⟨i>N⟨ i>,⟨i⟩Ô⟨ i>′-tridentate Schiff base ligand: synthesis, crystal structure and ⟨i>in vitro⟨ i> cytotoxicity. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 248-254. Catalytic H⟨sub>2⟨ sub> Evolution by a Mononuclear Cobalt Complex with a Macrocyclic		
9868	⟨i⟩O⟨ i⟩,⟨i⟩N⟨ i⟩,⟨i⟩€²-tridentate Schiff base ligand: synthesis, crystal structure and ⟨i⟩in vitro⟨ i⟩ cytotoxicity. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 248-254. Catalytic H⟨sub⟩2⟨ sub⟩ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139. A new tripodal kojic acid derivative for iron sequestration: Synthesis, protonation, complex formation studies with Fe3+, Al3+, Cu2+ and Zn2+, and in vivo bioassays. Journal of Inorganic	1.0	14
9868 9869	<i>>O</i> , <i>N</i> , <i>N</i> , <i>O</i> , <ii>Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 248-254. Catalytic H₂ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139. A new tripodal kojic acid derivative for iron sequestration: Synthesis, protonation, complex formation studies with Fe3+, Al3+, Cu2+ and Zn2+, and in vivo bioassays. Journal of Inorganic Biochemistry, 2019, 193, 152-165. Robust Entanglement Generation in Lithium Ions Mediated by Graphene Quantum Dots Interaction.</ii>	1.0	14
9868 9869 9870	<i>>O</i> , <i>N</i> , <i>O</i> , <i>O</i> , <i>O</i> , <i>O</i> , <i>O</i> , <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i i="" o<="">, <i< td=""><td>1.0 1.5 1.1</td><td>14 22 3</td></i<></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i></i>	1.0 1.5 1.1	14 22 3
9868 9869 9870 9871	<i>O</i> , <i>N</i> , <i>N</i> , <i>O</i> , <i>Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 248-254. Catalytic H sub> 2 Sub> Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139. A new tripodal kojic acid derivative for iron sequestration: Synthesis, protonation, complex formation studies with Fe3+, Al3+, Cu2+ and Zn2+, and in vivo bioassays. Journal of Inorganic Biochemistry, 2019, 193, 152-165. Robust Entanglement Generation in Lithium Ions Mediated by Graphene Quantum Dots Interaction. Journal of Physical Chemistry A, 2019, 123, 1790-1795. Synthesis, Spectroscopy, X-ray Crystallography, and DFT Studies of Dichlorobis[1-(allyl)-1H-imidazole-¹eN3] copper(II). Russian Journal of Physical Chemistry A, 2019, 93, 2758-2764. A density functional theory study on multiple exciton generation in lead chalcogenides. Molecular</i>	1.0 1.5 1.1	14 22 3
9868 9869 9870 9871 9872	⟨i⟩ ⟨i⟩,⟨i⟩,⟨i⟩,⟨i⟩,⟨i⟩ ′-tridentate Schiff base ligand: synthesis, crystal structure and ⟨i⟩ in vitro⟨ i⟩ cytotoxicity. Acta Crystallographica Section C, Structural Chemistry, 2019, 75, 248-254. Catalytic H⟨sub⟩ 2⟨ sub⟩ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139. A new tripodal kojic acid derivative for iron sequestration: Synthesis, protonation, complex formation studies with Fe3+, Al3+, Cu2+ and Zn2+, and in vivo bioassays. Journal of Inorganic Biochemistry, 2019, 193, 152-165. Robust Entanglement Generation in Lithium Ions Mediated by Graphene Quantum Dots Interaction. Journal of Physical Chemistry A, 2019, 123, 1790-1795. Synthesis, Spectroscopy, X-ray Crystallography, and DFT Studies of Dichlorobis[1-(allyl)-1H-imidazole-I®N3] copper(II). Russian Journal of Physical Chemistry A, 2019, 93, 2758-2764. A density functional theory study on multiple exciton generation in lead chalcogenides. Molecular Crystals and Liquid Crystals, 2019, 693, 57-65. New design of two series of Ir(â¢) complexes by changing substitute group at main ligand or ancillary	1.0 1.5 1.1 0.1 0.4	14 22 3 1

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