

Ramiro Arratia-Perez

rarratia@unab.cl

PUBLICATIONS 1983-2014

1. R. Arratia-Perez, D. A. Case
Relativistic effects on molecular hyperfine interactions: Application to XeF and CsO
J. Chem. Phys. 79, 4939-4949 (1983)
2. R. Arratia-Perez, D. A. Case
Electronic structure of octachloroditungstate(II)
Inorg. Chem. 23, 3271-3273 (1984)
3. C. Y. Yang, R. Arratia-Perez, J. P. Lopez
Electronic structure of tungsten hexacarbonyl
Chem. Phys. Lett. 107, 112-116 (1984)
4. R. Arratia-Perez, C. Y. Yang
Bonding in metal hexacarbonyls
J. Chem. Phys. 83, 4005-4015 (1985)
5. R. Arratia-Perez, G. L. Malli
Dirac scattered-wave calculations for Ag_{2+3} , Au_{q+3} , and Au_{q+4} ($q=1, 2$) clusters
J. Chem. Phys. 84, 5891-5897 (1986)
6. F. Zuloaga, R. Arratia-Perez
Metal scattered wave study of the relativistic and nonrelativistic electronic structure and bonding for cis-diamminedichloroplatinum(II)
J. Phys. Chem. 90, 4491-4499 (1986)
7. R. Arratia-Perez, G. L. Malli
Bonding in the octahedral Au_6^{2+} cluster
Chem. Phys. Lett. 125, 143-148 (1986)
8. R. Arratia-Perez, G. L. Malli
Dirac scattered-wave study of trigonal bipyramidal silver clusters Ag_5^{q+} ($q=0, 2-4$)
J. Chem. Phys. 85, 6610-6622 (1986)
9. A. Ramos, R. Arratia-Perez, G. L. Malli
Dirac scattered-wave calculations on an icosahedral Au_{13} cluster
Phys. Rev. B. Cond. Matt. 35, 3798 (1987)

10. R. Arratia-Perez, G. L. Malli
Bonding, optical, and magnetic properties of paramagnetic Ag_4^{1+} and Ag_4^{3+} clusters
J. Magn. Reson. 73, 134-142 (1987)
11. R. Arratia-Perez, F. U. Axe, D. S. Marynick
Geometry, bonding, optical, magnetic properties of $Cu(CO)_3$
J. Phys. Chem. 91, 5177-5183 (1987)
12. R. Arratia-Perez, D. S. Marynick
Molecular hyperfine interactions in $Ag(CO)_3$
J. Chem. Phys. 87, 4644-4650 (1987)
13. R. Arratia-Perez, D. S. Marynick
Paramagnetic resonance hyperfine structure of hexachloro protactinate
Phys. Rev. B, Cond. Matt. 37, 4893-4899 (1989)
14. R. Arratia-Perez, A. F. Ramos, G. L. Malli
Calculated electronic structure of Au_{13} clusters
Phys. Rev. B, Cond. Matt. 39, 3005-3009 (1989)
15. R. Arratia-Perez
Relativistic electronic structure of the staggered, eclipsed conformations of octachloro diosmate(III)
J. Phys. Chem. 95, 7239-7244 (1991)
16. R. Arratia-Perez
Relativistic quantum chemistry as a tool for calculating optical, spin-dependent properties of heavy metal clusters
Proc. Symp. Chemistry of Materials of Technological Interest, Pucón, Chile, Commission of the European Communities, Conicyt (1991)
17. R. Arratia-Perez, L. Hernandez-Acevedo
Spin-orbit effects on heavy metal octahedral clusters
J. Mol. Struct. THEOCHEM 282, 131-414 (1993)
18. R. Arratia-Perez
Spin-orbit effects on RuO_4 , OsO_4
Chem. Phys. Lett. 203, 409-414 (1993)
19. R. Arratia-Perez
The $M_6S_8L_6$ clusters: An example in cluster, condensed phase chemistry
Chem. Phys. Lett. 213, 547-553 (1993)
20. J. Pablo Bravo-Vasquez, R. Arratia-Perez
Calculated paramagnetic hyperfine structure of the C_{2v} isomers of Ag_3
J. Phys. Chem. 98, 5627-5631 (1994)

21. R. Arratia-Perez, L. Hernandez-Acevedo, J. S. Gomez-Jeria
Calculated paramagnetic properties of the matrix isolated Au₃ cluster
Chem. Phys. Lett. 236, 37-42 (1995)
22. R. Arratia-Perez, L. Hernandez-Acevedo
A Dirac molecular orbital study for encapsulated heavy transition metals within yttrium cluster iodides
Chem. Phys. Lett. 247, 163-167 (1995)
23. R. Arratia-Perez, L. Hernandez-Acevedo
A Dirac molecular orbital study for the tetragonal compression in the RuY₆I₁₂²⁻ cluster
Chem. Phys. Lett. 255, 217-222 (1996)
24. R. Arratia-Perez, L. Hernandez-Acevedo
A Dirac molecular orbital study for hexanuclear tungsten cluster structures
Chem. Phys. Lett. 277, 223-227 (1997)
25. R. Arratia-Perez, L. Hernandez-Acevedo, L. Alvarez-Thon
Calculated paramagnetic hyperfine structure of pentagonal bipyramid Ag₇ cluster
J. Chem. Phys. 108, 5795-5798 (1998)
26. R. Arratia-Perez, L. Hernandez-Acevedo
Calculated paramagnetic resonance parameters of a gallium arsenide cluster: Ga₂As₃
J. Chem. Phys. 109, 3497-3503 (1998)
27. R. Arratia-Perez, L. Hernandez-Acevedo
The hexanuclear rhenium cluster ions Re₆S₈X₆⁴⁻. Are these clusters luminescent?
J. Chem. Phys. 110, 2529-2532 (1999)
28. R. Arratia-Perez, L. Hernandez-Acevedo
Relativistic electronic structure of an icosahedral Au₁₂Pd cluster
Chem. Phys. Lett. 303, 641-646 (1999)
29. R. Arratia-Perez, L. Hernandez-Acevedo, B. Weiss-Lopez
Calculated paramagnetic resonance hyperfine structure of the acute GaAs₂, obtuse Ga₂As clusters
J. Chem. Phys. 110, 10882-10887 (1999)
30. R. Arratia-Perez, L. Hernandez-Acevedo
The Re₆Se₈Cl₄⁻⁶ and Re₆Se₈I₄⁻⁶ cluster ions: Another example of luminescent clusters?
J. Chem. Phys. 111, 168-172 (1999)
31. L. Alvarez-Thon, L. Hernandez-Acevedo, R. Arratia-Perez
Calculated paramagnetic resonance parameters of the luminescent Re₆Se₈Cl₆³⁻ cluster ion.
J. Chem. Phys. 115, 726-730 (2001)

32. R. Arratia-Perez, L. Hernandez-Acevedo
Calculated paramagnetic resonance parameters (g, A_{hi}) of the Re₆S₈Br₃⁻⁶, Re₆S₈I₃⁻⁶, and Re₆Se₈I₃⁻⁶ cluster ions
J. Chem. Phys. 118, 7425-7430 (2003)
33. L. Hernandez-Acevedo, R. Arratia-Perez
Relativistic electronic structure of molecular precursors: The case of the [Re₆Q₈(CN)₆]⁴⁻/[Re₆Q₈(CN)₆]³⁻ (Q = S, Se) redox couples.
J. Chil. Chem. Soc. 48, 125 (2003)
34. R. Sienna Muraña, L. Hernandez-Acevedo, R. Arratia-Perez
Electronic structure, bonding of the [W₆S₈(CN)₆]⁶⁻ cluster anion
Chem. Phys. Lett. 393, 277-281 (2004)
35. R. Arratia-Perez, L. Alvarez-Thon, P. Fuentealba
Calculated geometry, paramagnetic hyperfine structure of the Cu₇ cluster
Chem. Phys. Lett. 397, 408-411 (2004)
36. R. Arratia-Perez, L. Hernandez-Acevedo, G. L. Malli
Calculated optical, magnetic properties of hexafluorouranate (V) anion: UF₆⁻
J. Chem. Phys. 121, 7743-7747 (2004)
37. L. Hernandez-Acevedo, R. Arratia-Perez
Spin-orbit effects in metal-metal multiple bonded M₂X₂ halide complexes
J. Chil. Chem. Soc. 49, 361-365 (2004)
38. R. Arratia-Perez, G. L. Malli
Relativistic molecular orbital study of the optical, magnetic properties of hexachloro protactinate (IV): PaCl₆²⁻
J. Chem. Phys. 124, 074321 (2006)
39. J. David, F. Mendizabal, R. Arratia-Perez
Electronic structure, molecular properties of the heptacyanorhenate [Re(CN)₇]³⁻, [Re(CN)₇]⁴⁻ complexes.
J. Phys. Chem. A 110, 1072-1077 (2006)
40. J. David, F. Mendizabal, R. Arratia-Perez
Electronic structure, molecular properties of the octacyanorhenate [Re(CN)₈]³⁻ and [Re(CN)₈]²⁻ complexes.
Chem. Phys. Lett. 422, 89-94 (2006)
41. D. MacLeod C. A. Muñoz-Castro, C. J. Bustos, J. M. Manriquez, R. Arratia-Perez
p-Donor/Acceptor Effect on Lindqvist type polyoxomolibdates because of various multiple-bonded nitrogeneous ligands
J. Phys. Chem. A 111, 6563-6567 (2007)

42. L. Alvarez-Thon, J. David, R. Arratia-Perez, K. Seppelt
Ground state of octahedral platinum hexafluoride
Phys. Rev. A 77, 034502-1- 034502-4 (2008)
43. R. Ramirez-Tagle, R. Arratia-Perez
The luminescent $[Mo_6X_8(NCS)_6]^{2-}$ ($X = Cl, Br, I$) Clusters?: A computational study based on time-dependent density functional theory including spin-orbit and solvent-polarity effects
Chem. Phys. Lett. 455, 38-41 (2008)
44. R. Ramirez-Tagle, R. Arratia-Perez
Electronic structure, molecular properties of the $[Mo_6X_8L_6]^{2-}$; $X = Cl, Br, I$; $L = F, Cl, Br, I$ clusters
Chem. Phys. Lett. 460, 438-441 (2008)
45. P. J. Orto, G. S. Nichol, N. Okumura, D. H. Evans, R. Arratia-Perez, R. Ramirez-Tagle, R. Wang, Z. Zheng
Cluster carbonyls of the $[Re_6(m3-Se)_8]^{2+}$ core: synthesis, structural characterization, computational analysis
Dalton Trans. 4247-4253 (2008)
46. L. Alvarado-Soto, R. Ramirez-Tagle, R. Arratia-Perez
Spin-orbit effects on the aromaticity of the Re_3Cl_9, Re_3Br_9 clusters
Chem. Phys. Lett. 467, 94-96 (2008)
47. R. Ramirez-Tagle, R. Arratia-Perez
Electronic Structure and Molecular Properties of the Mixed Rhenium-Molybdenum $[Re_6^xMo_xS_8(CN)_6]^{q-}$, ($x = 0$ to 6) Clusters
J. Clust. Sci. 20, 159-164 (2009)
48. F. Araneda, S. Salinas, D. MacLeod-Carey, A. Muñoz-Castro, R. Arratia-Perez, C. Adams, I. Chavez, J. M. Manriquez
Synthesis, characterization of a new carbonylated Zirconium metallocene using a dichloro-zirconocene derived from partially alkylated s-indacene
J. Chil. Chem. Soc. 54, 269-273 (2009)
49. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez
Electronic Structure, Molecular Properties of Binuclear Group VII Pentalene Metal Carbonyl Complexes $[C_8H_6\{M(CO)_3\}_2]$ ($M = Mn, Tc, Re, Bh$): A Relativistic Density Functional Theory Study
Polyhedron 28, 1561-1567 (2009)
50. L. Alvarez-Thon, R. Arratia-Perez, K. Seppelt
Comments on Ground state of octahedral platinum hexafluoride
Phys. Rev. A, 79, 056502-056503 (2009)

51. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez
Electronic Structure, molecular properties, Electronic currents of the luminescent [Au₃(CH₃N=COCH₃)₃] cluster
Chem. Phys. Lett. 474, 290-293 (2009)
52. L. Alvarado-Soto, R. Ramirez-Tagle, R. Arratia-Perez
Spin-orbit effects on Re₃X₉²⁻ cluster ions
J. Phys. Chem. A (Letters) 113, 1671-1673 (2009)
53. J. Hurtado, D. MacLeod-Carey, A. Muñoz-Castro, R. Arratia-Perez, R. Quijada, Guang Wu, R. Rojas, M. Valderrama
Chromium(III) complexes with terdentate 2,6-bis(azolylmethyl)pyridine ligands: synthesis, structures, catalytic behavior
J. Organomet. Chem. 694, 2636-2641 (2009)
54. R. Ramirez-Tagle, R. Arratia-Perez
Pyridine as axial ligand on the [Mo₆Cl₈]⁴⁺ core switches off luminescence
Chem. Phys. Lett. 475, 232-234 (2009)
55. A. Muñoz, D. MacLeod-Carey, R. Arratia-Perez
Relativistic electronic structure of Cadmium(II) multidecker phthalocyanine compounds
Polyhedron 29, 451-455 (2010)
56. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez
Calculated Molecular Properties of triangular Tribenzo, Perfluoro-ribenzo Trimercuric Macrocycles
J. Phys. Chem. A, 114, 666-672 (2010)
57. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez
Inside of a Superatom. The M₇^q (M = Cu, Ag, q = 1+, 0, 1-) case
Chem. Phys. Phys. Chem, 11, 646-650 (2010)
58. D. Paez-Hernandez, R. Ramirez-Tagle, E. Codorniu-Hernandez, L. A. Montero-Cabrera, R. Arratia-Perez
Quantum relativistic investigation about the coordination, bonding effects of different ligands on uranyl complexes
Polyhedron 29, 975-984 (2010)
59. X. Tu, E. Boroson, H. Truong, A. Muñoz-Castro, R. Arratia-Perez, G. S. Nichol, Z. Zheng
Cluster-Bound Nitriles Do Not Click with Organic Azides: Unexpected Formation of Imino Complexes of the [Re₆(^β-Se)₈]²⁺ Core-Containing Clusters
Inorg. Chem. 49, 380-382 (2010)

60. D. MacLeod-Carey, C. Morales-Verdejo, A. Muñoz-Castro, F. Burgos, D. Abril, C. Adams, E. Molins, O. Cador, I. Chavez, J. M. Manriquez, R. Arratia-Perez, J. Y. Saillard *[Cp*Ru(s-indacene)RuCp*], [Cp*Ru(s-indacene)RuCp*]⁺: Experimental, theoretical findings concerning the electronic structure of neutral, mixed valence organometallic systems*
Polyhedron 29, 1137-1143 (2010)
61. R. Ramirez-Tagle, L. Alvarado-Soto, L. Hernandez-Acevedo, R. Arratia-Perez *Spin-orbit, solvent effects in the luminescent [Re₆Q₈(NCS)₆]⁴⁺, Q = S, Se, Te clusters: Molecular sensors, Molecular devices*
J. Chil. Chem. Soc. 55, 39-43 (2010)
62. A. Muñoz-Castro, D. MacLeod-Carey, C. Morales-Verdejo, I. Chavez J. M. Manriquez, R. Arratia-Perez
Toward the synthetic control of the HOMO-LUMO Gap in Binuclear systems. Insights from Density Functional Calculations
Inorg. Chem. 49, 4175-4178 (2010)
63. A. Muñoz-Castro, R. Arratia-Perez
Electronic Delocalization, Energetics, Optical Properties of Tripalladium Ditropylium Halides, [Pd₃(C₇H₇)₂X₃]¹⁻ (X) Cl⁻, Br⁻, I
J. Phys. Chem. A 114, 5217-5221 (2010)
64. R. S. Chauhan, G. Kedarnath, A. Wadawale, A. Muñoz-Castro, R. Arratia-Perez, V. K. Jain, W. Kaim
Tellurium(0) as a Ligand: Synthesis and Characterization of 2-Pyridyltellurolates of Platinum(II) and Structures of [Pt{2-Te-3-(R)C₅H₃N₂}₂Te(PR'₃)] (R = H or Me)
Inorg. Chem. 49, 4179-4185 (2010)
65. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez
Spin-orbit effects on electronic delocalization. Aromaticity in a discrete square tetrapalladium sandwich complex
J. Chem. Phys. 132, 164308 (2010)
66. R. Veloso-Bahamonde, R. Ramirez-Tagle, R. Arratia-Perez
DFT-modeling of the tungsten (V) cofactor of hyperthermophilic Pyrococcus furiosus tungsto-bispterin enzyme via the calculated EPR Parameters
Chem. Phys. Lett. 491, 214-217 (2010)
67. D. Sierra, A. Hugo Klahn, R. Ramirez-Tagle, R. Arratia-Perez, F. Godoy, M. T. Garland, M. Fuentealba
Heterobimetallic Re=Pd complexes bridged by η¹:η⁵-Ph₂PC₅H₄ ligand. Synthesis, electronic and crystal structure of (CO)₂(PR₃)(η⁵-C₅H₄PPh₂)Re-PdCl₂, R = Me and OMe
Dalton Trans. 39, 6295-6301 (2010)

68. V. Nguyen-Duc, I. Tiritiris, R. F. Winter, B. Sarkar, P. Singh, C. Duboc, A. Muñoz-Castro, R. Arratia-Perez, W. Kaim, T. Schleid
Oxidative Perhydroxylation of [closob-B₁₂H₁₂]²⁻ to the Stable Inorganic Cluster Redox System [B₁₂(OH)₁₂]^{2-/-}: Experiment and Theory
Chemistry, A Eur. Journal 16, 11242-11245 (2010)
69. X. Zarate, E. Schott, D. MacLeod-Carey, C. Bustos, R. Arratia-Perez,
DFT study on the electronic structure, energetics, spectral properties of several bis(organohydrazido(2-)) molybdenum complexes containing substituted phosphines, chloro atoms as ancillary ligands
J. Mol. Struct. THEOCHEM 957, 126-132 (2010)
70. X. Tu, E. Alster, A. Muñoz-Castro, R. Arratia-Perez, G. S. Nichol, Z. Zheng
Geometrically Specific Imino Complexes of the [Re₆(3-Se)₈]⁷⁺ Core-Containing Clusters
Chem. Eur. J. 17, 580–587 (2011)
71. M. Sancy, J. Pavez, M. A. Gulppi, I. L. de Mattos, R. Arratia-Perez, C. Linares-Flores, M. Paez, T. Nyokong, J. H. Zagal
Optimizing the Electrocatalytic Activity of surface confined Co Macrocycles For the Electrooxidation of Thiocyanate at pH 4
Electroanalysis 23, 711-718 (2011)
72. F. Ferraro, R. Arratia-Perez
Spin-orbit effects on the Optical, Magnetic Properties of Cerium (III) Hexahalides
Polyhedron 30, 860-863 (2011)
73. X. Zarate, E. Schott, R. Arratia-Perez
A DFT/TDDFT Study of Porphyrazines, Phthalocyanine Oxo-Titanium Derivatives as Potential Dyes in Solar Cells
Int. J. Quantum Chem. 111, 4186-4196 (2011)
74. E. Schott, X. Zarate, R. Arratia-Perez
Relativistic scalar, spin-orbit density functional calculations of the electronic structure, NICS index, ELF function of the [Re₂(CO)₈(μ -BiPh)₂], [Re₂(CO)₈(μ-BiPh₂)] clusters
Polyhedron 30, 846-850 (2011)
75. L-C. Pop, D. MacLeod-Carey, A. Muñoz-Castro, L. Silaghi-Dumitrescu,, A. Castel, R. Arratia-Perez
Relativistic Calculations of Aminotroponimate complexes containing group 15 (P, As, Sb, Bi) elements
Polyhedron 30, 841-845 (2011)
76. M. T. Garland, S. Kahlal, D. MacLeod-Carey, R. Arratia-Perez, J. M. Manriquez, J-Y. Saillard
Electronic structure, metal–metal communication in (CpM)₂(as-indacene), (CpM)₂(s-indacene) (M = Mn, Fe, Co, Ni) complexes: a DFT investigation
New J. Chem. 35, 2136-2145 (2011)

77. A. Carreño, E. Schott, X. Zarate, R. Arratia-Perez, J. C. Vega, M. Mardones, J. M. Manriquez, I. Chavez
Adsorption essays of Palladium in Modified Silica Gel with Thioureonium groups: Experimental, Theoretical Studies
J. Chil. Chem. Soc. 56, 692-696 (2011)
78. D. Paez-Hernandez, J. A. Murillo-Lopez, R. Arratia-Perez
Bonding Nature, Electron Delocalization of An(COT)₂, An = Th, Pa, U
J. Phys. Chem. A 115, 8997-9003 (2011)
79. R. Ramirez-Tagle, L. Alvarado-Soto, R. Arratia-Perez, R. Bast, L. Alvarez-Thon
Probing the aromaticity of the [(H_iAc)₃(μ₂-H)₆], [(H_iTh)₃(μ₂-H)₆]⁺, and [(H_iPa)₃(μ₂-H)₆] clusters
J. Chem. Phys. 135, 104506-8 (2011)
80. I. Ponce, J. F. Silva, R. Onate, S. Miranda-Rojas, A. Munoz-Castro, R. Arratia-Perez, F. Mendizabal, J. H. Zagal
Theoretical, Experimental Study of Bonding, Optical Properties of Self-Assembly Metallophthalocyanines Complexes on a Gold Surface. A Survey of the Substrate-Surface Interaction
J. Phys. Chem. C. 115, 23512-23518 (2011)
81. J. Hurtado, J. Ugarte, R. Rojas, M. Valderrama, D. MacLeod-Carey, A. Muñoz-Castro, R. Arratia-Perez, R. Fröhlich
New bis(azolylcarbonyl)pyridine chromium(III) complexes as initiators for ethylene polymerization
Inorg. Chim. Acta 378, 218-223 (2011)
82. A. Muñoz-Castro, R. Arratia-Perez
Spin-Orbit effects on a Gold-Based Superatom: A Relativistic Jellium Model
Phys. Chem. Chem. Phys. 14, 1408-1411 (2012)
83. D. Paez-Hernandez, R. Arratia-Perez
Charge transfer effects on the paramagnetic properties of the [M(C₈H₈)₂] and M(C₃H₅)(C₈H₈); M = Ti, Zr, Hf and Th, complexes
Polyhedron 36, 69-72 (2012)
84. X. Zarate, E. Schott, D. MacLeod-Carey-Castro, R. Arratia-Perez
Photophysical properties of [Cu(binap)₂]⁺, [Pd(binap)₂] complexes: a theoretical study
Polyhedron 37, 54-59 (2012)
85. E. Schott, X. Zarate, R. Arratia-Perez
Electronic Structure, Molecular Properties of Paramagnetic Hexanuclear Tantalum [Ta₆X₁₂Y₆]³⁻ (X, Y= F, Cl, Br, I) Cluster Compounds
Polyhedron 36, 127-132 (2012)

86. R. Singh Chauhan, G. Kedarnath, A. Wadawale, A. L. Rheingold, A. Muñoz-Castro, R. Arratia-Perez, V. K. Jain
Reactivity of dipyridyl ditellurides with (diphosphine)PtO, 2-pyridyltellurolates with (diphosphine)PtCl₂, isolation of different structural motifs of platinum(II) complexes
Organometallics 31, 1743-1750 (2012)
87. A. Muñoz-Castro, D. MacLeod-Carey, R. Arratia-Perez, G. L. Malli
Relativistic effects in bonding, isomerization energy of the superheavy roentgenium (111Rg) cyanide
Polyhedron 39, 113-117 (2012)
88. C. Linares-Flores, D. MacLeod-Carey, A. Muñoz-Castro, J. H. Zagal, J. Pavez, D. Pino-Riffo, R. Arratia-Perez
Reinterpreting the role of the catalyst formal potential. The case of thiocyanate electrooxidation catalyzed by CoN₄-Macrocyclic complexes
J. Phys. Chem. C. 116, 7091-7098 (2012)
89. F. Ferraro, C. Aparecida Barboza, R. Arratia-Perez
A Relativistic Study of the Electronic, Magnetic Properties of Cerocene, Thorocene, its Anions
J. Phys. Chem. A. 116, 4170- 4175 (2012)
90. C. Echeverria, A. Becerra, F. Nuñez-Villena, A. Muñoz-Castro, J. Stehberg, Z. Zheng, R. Arratia-Perez, F. Simon, R. Ramirez-Tagle
The paramagnetic, luminescent [Re₆Se₈I₆]³⁻ cluster. Its potential use as an antitumoral, biomarker agent
New J. Chem, 36, 927-932 (2012)
91. C. A. Barboza, R. Arratia-Perez, D. MacLeod-Carey
Theoretical study of 3, 3' substitution of 9,9,9',9'-tetramethyl-fluorene-dimers
Chem. Phys. Lett. 538, 67-71 (2012)
92. C. A. Barboza, P. A. M. Vazquez, D. MacLeod-Carey, R. Arratia-Perez
A TDDFT Basis Set, Functional Assessment for the Calculation of Electronic Excitation Energies of Fluorenes.
Int. J. Quantum Chem. 112, 3434-3438 (2012)
93. C. A. Barboza, E. Barboza, D. MacLeod-Carey, R. Arratia-Perez
Methylation, the system-size effect over the structural, electronic, magnetic (NICS), reactive properties of pentalene derivatives
Chem. Phys. Lett. 545, 88-94, (2012)
94. D. Paez-Hernandez; R. Arratia-Perez
Aromaticity, Optical Properties and Zero Field Splitting of Homo- and Hetero-bimetallic (C₈H₈)M(μ₂-, η⁸=C₈H₈)M(C₈H₈) where M = Ti, Zr, Th Complexes
J. Phys. Chem. A 116 (28), 7584–7592 (2012)

95. E. Schott, X. Zarate, R. Arratia-Perez
Substituents Effects on Two Related Families of Dyes for Dye Sensitized Solar Cells: $[\text{Ru}(4,4'\text{-R,R-2,2'\text{-bpy}})_3]^{2+}$ and $[\text{Ru}(4,4'\text{-COOH-2,2'\text{-bpy}})(4,4'\text{-R,R-2,2'\text{-bpy}})_2]^{2+}$
J. Phys. Chem. A 116 (27), 7436–7442 (2012)
96. I. Ponce, J. F. Silva, R. Oñate, M. Caroli Rezende, M. A. Paez, J. H. Zagal, J. Pavez, F. Mendizabal, S. Miranda-Rojas, A. Muñoz-Castro, R. Arratia-Perez
Enhancement of the Catalytic Activity of Fe Phthalocyanine for the Reduction of O₂ Anchored to Au(111) via Conjugated Self-Assembled Monolayers of Aromatic Thiols compared to Cu Phthalocyanine
J. Phys. Chem. C 116 (29), 15329–15341 (2012)
97. D. MacLeod-Carey, C. Adams, A. Muñoz-Castro, C. Morales-Verdejo, J. F. Araneda, I. Martinez, I. Chavez, J. M. Manriquez, A. Castel, P. Rivière, M. Rivière-Baudet, D. Matioszek, R. Septelean, I. Martinez, R. Arratia-Perez,
A new method to radical anions derived from s-Indacene organobimetallic complexes, their ESR characterization
Inorg. Chim. Acta 392, 154-159 (2012)
98. L. Alvarado-Soto, E. Schott V, X. Zarate, R. Arratia-Perez, R. Ramirez-Tagle
The aromaticity of the $[\text{Re}_3(\mu\text{-X})_3\text{X}_9]^{3-}$ clusters, X= Cl, Br, I
Chem. Phys. Lett. 545, 50-53 (2012)
99. D. Paez-Hernandez, J. Murillo-Lopez, R. Arratia-Perez
Optical, magnetic properties of bis (dicyclooctatetraenyl) diuranium complex. A theoretical view
Organometallics 31, 6297-6304 (2012)
100. B. Oviedo, X. Zarate, C. F. A. Negre, E. Schott, R. Arratia-Perez, C. G. Sanchez
Quantum Dynamical Simulations as a Tool for Predicting Photoinjection Mechanisms in Dye-sensitized TiO₂ Solar Cells.
Phys. Chem. Lett. 3, 2548-2555 (2012)
101. F. Ferraro, R. Arratia-Perez
Bonding, Energetic, Electronic Delocalization, Optical Properties of MCp_3 Complexes, where M = Sc, Y, La, Ac, Lu, Ce, Yb, Th
Chem. Phys. Lett. 554, 219-224 (2012)
102. D. A. Geraldo, N. Arancibia-Miranda, N. A. Villagra, G. C. Mora, R. Arratia-Perez
Synthesis of CdTe QDs/single-walled aluminosilicate nanotubes hybrid compound, their antimicrobial activity on bacteria
J. Nanopart. Res. 14, 1286-1294 (2012)
103. A. Trujillo, M. Fuentealba, R. Arratia-Perez, J. A. K. Howard
trans-Bis[1,2-bis(diphenylphosphanyl)ethane]chlorido(ethynyl)ruthenium(II)
Acta Cryst. E68, m1445 (2012)

104. X. Zarate, E. Schott, R. Arratia-Perez
Effects of the peripheral substituents (-NH₂, -OH, -CH₃, -H, -C₆H₅, -Cl, -CO₂H, -NO₂) on molecular properties of a Ni-Porphyrzine dimers family
Polyhedron 50, 131-138 (2013)
105. C. Morales-Verdejo, L. Oehninger, I. Martinez-Diaz, D. MacLeod-Carey, R. Arratia-Perez, I. Chavez, J. M. Manriquez
A New heterobimetallic manganese-rhodium carbonyl complex derived from partially alkylated s-indacene
Inorg. Chim. Acta 394, 132-139 (2013)
106. X. Zarate, E. Schott, T. Gomez, R. Arratia-Perez
A Theoretical Study of Sensitizer Candidates for Dye-Sensitized Solar Cells: Peripheral Substituted Di-Zn-Pyrazinoporphyrazine-Phthalocyanine Complexes
J. Phys. Chem. A 117, 430-438 (2013)
107. E. Schott, X. Zarate, R. Arratia-Perez
Molecular Properties of Two Related Families of Substituted [Ru(2,2':6',2''-Terpyridine)₂]²⁺ for Application as Sensitizers in Dye-Sensitized Solar Cells
Dyes, Pigments 97, 455-461 (2013)
108. L. Oehninger, J. F. Araneda, C. Morales-Verdejo, A. Munoz-Castro, D. MacLeod-Carey, C. Adams, R. Arratia-Perez, R. Rojas, J. M. Manriquez, I. Chavez,
Novel titanocene derived from a partially alkylated s-indacene: Synthesis, characterization, comparative study with its zirconium analog
Inorg. Chim. Acta 396, 35-39 (2013)
109. E. Schott, X. Zarate, D. MacLeod-Carey, R. Arratia-Perez, C. Bustos
Substituents effect on the electronic structure, molecular properties of bis[organohydrazido(2-)] molybdenum(VI) complexes
Polyhedron 61, 27-32 (2013)
110. F. Ferraro, D. Paez-Hernandez, J. A. Murillo-Lopez, A. Muñoz-Castro, R. Arratia-Perez
Antenna Effect by Organometallic Chromophores in Bimetallic d-f Complexes
J. Phys. Chem. A 117, 7847-7854 (2013)
111. S. Miranda-Rojas, A. Munoz-Castro, R. Arratia-Perez, F. Mendizabal
Theoretical insights into the adsorption of neutral, radical, anionic thiophenols on gold(111)
Phys. Chem. Chem. Phys. 15, 20363 (2013)
112. F. Miranda-Barrientos, A. Muñoz-Castro, R. Arratia-Perez, D. MacLeod-Carey,
Theoretical Calculations of an Osmium Molecular Switch
J. Chil. Chem. Soc. 58, 2110-2113 (2013)

113. W. Rabanal-Leon, R. Arratia-Perez
Relativistic DFT study of the Electronic Structure of the [ReF₈]⁻ and [UF₈]²⁻ Ions
J. Chil. Chem. Soc. 58, 2020-2024 (2013)
114. C. Morales-Verdejo, I. Martinez-Diaz, C. Adams, J. F. Araneda, L. no Oehninger, D. MacLeod-Carey, A. Muñoz-Castro, R. Arratia-Perez, I. Chavez, J. M. Manriquez
New mono, bimetallic iron complexes derived from partially methylated s-indacene. Evidence of a trinuclear iron s-indacene complex
Polyhedron 69, 15-24 (2014)
115. C. D. McTiernan, E. I. Alarcon, G. L. Hallett-Tapley, J. Murillo-Lopez, R. Arratia-Perez, J. C. Netto-Ferreira, J. C. Scaiano
Electron transfer from the benzophenone triplet excited state directs the photochemical synthesis of gold nanoparticles
Photochemical & Photobiological Sciences, 13, 149-153 (2014)
116. K. Hu, K. C. D. Robson, E. E. Beauvilliers, E. Schott, X. Zarate, R. Arratia-Perez, C. P. Berlinguette, G. J. Meyer
Intramolecular, Lateral Intermolecular Hole Transfer at the Sensitized TiO₂ Interface
J. Am. Chem. Soc. 136, 1034-1046 (2014)
117. T. Gomez, X. Zarate, E. Schott, R. Arratia-Perez
Role of the main adsorption modes in the interaction of a dye-sensitized solar cell [COOH-TPP-Zn(II)] on the periodic TiO₂ slab exposing rutile (110) surface
RSC Advances 4, 9639-9646 (2014)
118. K. Hu, H. A. Severin, B. D. Koivisto, K. C. D. Robson, E. Schott, R. Arratia-Perez, G. J. Meyer, C. P. Berlinguette
Direct Spectroscopic Evidence for Constituent Heteroatoms Enhancing Charge Recombination at a TiO₂-Ruthenium Dye Interface
J. Phys. Chem. C 118, 17079-17089 (2014)
119. C. Linares-Flores, J. Espinoza-Vergara, J. H. Zagal, R. Arratia-Perez
Reactivity trends of Fe phthacyanines confined on graphite electrodes in terms of donor-acceptor intermolecular hardness: Linear versus Volcano Correlations
Chem. Phys. Lett. 614, 176-180 (2014)
120. W. A. Rabanal-Leon, D. Paez-Hernandez, R. Arratia-Perez
Covalent lanthanide(III) macrocyclic complexes: the bonding nature, optical properties of a promising single antenna molecule
Phys. Chem. Chem. Phys. 16, 25978-25998 (2014)
121. W. A. Rabanal-Leon, J. A. Murillo-Lopez, D. Paez-Hernandez, R. Arratia-Perez
Understanding the Influence of Terminal Ligands on the Electronic Structure, Bonding Nature in [Re₆(μ₃-Q₈)]²⁺ Clusters
J. Phys. Chem. A 118 (46), 11083-11089 (2014)