

IOAN SILAGHI-DUMITRESCU
1950-2009

Ioan Silaghi-Dumitrescu - List of Publications

Binuclear cyclopentadienylcobalt sulfur and phosphinidene complexes Cp₂Co₂E₂ (E = S, PX): Comparison with their Iron carbonyl analogues, Li, Guoliang; Li, Qian-Shu; Silaghi-Dumitrescu, Ioan; King, Bruce R.; Schaefer, Henry F, *Journal of Organometallic Chemistry* (2010), 695(6), 804-808.

On the microwave-assisted synthesis of acylphenothiazine derivatives- Experiment versus theory synergism, Gaina, Luiza; Porumb, Dan; Silaghi-Dumitrescu, Ioan; Cristea, Castelia; Silaghi-Dumitrescu, Luminita, *Canadian Journal of Chemistry* (2010), 88(1), 42-49.

(Diethylenetriamine)bis(theophyllinato)zinc(II) dihydrate. Mihaly, Bela; Forizs, Edit; Kun, Attila-Zsolt; Silaghi-Dumitrescu, Ioan, *Acta Crystallographica, Section E: Structure Reports Online* (2009), E65(5), m579.

An insight into the structure of model germaphosphaallenes, Petrar, P. M.; Nemes, G.; Silaghi-Dumitrescu, I.; Escudie, J.; Ranaivonjatovo, *Molecular Physics* (2009), 107(8-12), 1161-1167

Butterfly and rhombus structures for binuclear cobalt carbonyl sulfur and phosphinidene complexes of the type Co₂(CO)₆E₂ (E = S, PX), Li, Guoliang; Li, Qian-Shu; Silaghi-Dumitrescu, Ioan; King, R. Bruce; Schaefer, Henry F., III, *Dalton Transactions* (2009), (47), 10474-10480.

Endohedral Nickel, Palladium, and Platinum Atoms in 10-Vertex Germanium Clusters: Competition between Bicapped Square Antiprismatic and Pentagonal Prismatic Structures, King, R. B.; Silaghi-Dumitrescu, I.; Uta, M. M, *Journal of Physical Chemistry A* (2009), 113(3), 527-533.

From closo to isocloso structures and beyond in cobaltaboranes with 9 to 12 vertices, King R Bruce; Silaghi-Dumitrescu Ioan; Sovago Ioana, *Inorganic chemistry* (2009), 48(21), 10117-25.

Kinetic versus thermodynamic isomers of the deltahedral cobaltadiboraboranes, King R Bruce; Silaghi-Dumitrescu Ioan; Sovago Ioana, *Inorganic chemistry* (2009), 48(12), 5088-95.

N,N' and N,O chelated phosphonium cations containing aminotroponimate or aminotroponate units, Pop, Lucian-Cristian; Katir, Nadia; Castel, Annie; Silaghi-Dumitrescu, Luminita; Delpech, Fabien; Silaghi-Dumitrescu, Ioan; Gornitzka, Heinz; MacLeod-Carey, Desmond; Saffon, Nathalie, *Journal of Organometallic Chemistry* (2009), 694(9-10), 1562-1566.

Narrow-rim alkenyl calix[n]arene. Synthesis and spectral characterization, Saponar, Alina; Popovici, Elisabeth-Jeanne; Popovici, Nicolae; Bica, Ecaterina; Nemes, Gabriela; Petrar, Petronela; Silaghi-Dumitrescu, Ioan, *Revista de Chimie* (2009), 60(3), 278-282.

IOAN SILAGHI-DUMITRESCU
1950-2009

Stabilisation of an inorganic digallane by the phosphinobisthiolato P,S,S pincer ligand PPh(2-SC₆H₄)₂, Valean, Ana-Maria; Gomez-Ruiz, Santiago; Loennecke, Peter; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Hey-Hawkins, Evamarie, *New Journal of Chemistry* (2009), 33(8), 1771-1779.

The unique palladium-centered pentagonal antiprismatic cationic bismuth cluster: a comparison of related metal-centered 10-vertex pnictogen cluster structures by density functional theory, King R B; Silaghi-Dumitrescu I; Uta M M, *Inorganic chemistry* (2009), 48(17), 8508-14.

Lower Rim Silyl Substituted Calix[8]Arenes, Fleuret, Nathan; Paic, Sebastian; Nemes, Gabriela; Septelean, Raluca; Petrar, Petronela; Silaghi-Dumitrescu, Ioan, *Studia Universitatis Babes-Bolyai, Chemia* (2009), 54(3), 81-88.

Theoretical aspects of main group multiple bonded systems, Silaghi-Dumitrescu, Ioan; Petrar, Petronela; Nemes, Gabriela; King, R. Bruce, *Computational Inorganic and Bioinorganic Chemistry* (2009), 563-575.

vic-Dichlorodiphosphapropenes - synthesis and coordination ability, Septelean, Raluca; Nemes, Gabriela; Escudie, Jean; Silaghi-Dumitrescu, Ioan; Ranaivonjatovo, Henri; Petrar, Petronela; Gornitzka, Heinz; Silaghi-Dumitrescu, Luminita; Saffon, Nathalie, *European Journal of Inorganic Chemistry* (2009), (5), 628-634.

Beyond the icosahedron: a density functional theory study of 14-atom germanium clusters, King, R. Bruce; Silaghi-Dumitrescu, Ioan; Uta, Matei M, *European Journal of Inorganic Chemistry* (2008), (25), 3996-4003.

Beyond the Wade-Mingos Rules in Bare 10- and 12-Vertex Germanium Clusters: Transition States for Symmetry Breaking Processes, King, R. B.; Silaghi-Dumitrescu, I.; Uta, M. M, *Journal of Chemical Theory and Computation* (2008), 4(1), 209-215.

Bis(phosphanylamino)benzene ligands: a zinc(II) complex and an unusual nickel(I) complex with a Dewar-benzene-type Ni₂P₂N₂ backbone, Majoum-Mbe, F.; Kuehl, O.; Loennecke, P.; Silaghi-Dumitrescu, I.; Hey-Hawkins, E, *Dalton Transactions* (2008), (23), 3107-3114.

Germanium cluster polyhedral, Silaghi-Dumitrescu, Ioan; King, Bruce, *Studia Universitatis Babes-Bolyai, Chemia* (2008), 53(2), 83-88.

Interplay among Tetrahedrane, Butterfly Diradical, and Planar Rhombus Structures in the Chemistry of the Binuclear Iron Carbonyl Phosphinidene Complexes Fe₂(CO)₆(PX)₂, Silaghi-Dumitrescu, Ioan; Bitterwolf, Thomas E.; King, R. Bruce, *Journal of the American Chemical Society* (2008), 130(3), 901-906.

Palladium(II) and Platinum(II) Complexes with Heteroditopic 10-(Aryl)phenoxarsine (Aryl = 2-C₆H₄OR, R = H, Me, Pri) Ligands: Solvent-Oriented Crystallization of cis Isomers, Moldovan, Natalia; Loennecke, Peter; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Hey-Hawkins, Evamarie, *Inorganic Chemistry* (2008), 47(5), 1524-1531.

Polyhedral structures with three-, four-, and five fold symmetry in metal-centered ten-vertex germanium clusters, King R Bruce; Silaghi-Dumitrescu Ioan; Uta Matei-Maria (2008), 14(15), 4542-50.

IOAN SILAGHI-DUMITRESCU
1950-2009

Process for preparation of calixarene derivatives for the extraction of rare earth metal ions, Ursales, Traian; Popovici, Nicolae; Popovici, Elisabeth-Jeanne; Silaghi-Dumitrescu, Ioan; Palibroda, Nicolae. 121691 B1 20080228 Patent written in Romanian. Application: RO 2003-200300816 20031003. Priority: CAN 150:35528 AN 2008:361932.

Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-substituted derivatives of 2-aminopropane-1,3-diols, Pinteá, Monica; Fazekas, Marijana; Lameiras, Pedro; Cadis, Ionut; Berghian, Camelia; Silaghi-Dumitrescu, Ioan; Popa, Flavia; Bele, Constantin; Ple, Nelly; Darabantu, Mircea, *Tetrahedron* (2008), 64(37), 8851-8870.

Synthesis and characterisation of some copper oxide catalysts for ozone decomposition, Dan, C.; Popovici, E.-J.; Imre-Lucaci, F.; Popovici, N.; Marginean, P.; Silaghi-Dumitrescu, I, *Journal of Optoelectronics and Advanced Materials* (2008), 10(9), 2234-2236.

Temperature induced rotation in a [4.4]cyclophane, Bogdan, Niculina D.; Condamine, Eric; Toupet, Loic; Ramondenc, Yvan; Silaghi-Dumitrescu, Ioan; Grosu, Ion, *Tetrahedron Letters* (2008), 49(35), 5204-5207. **Abstract**

The role of "external" lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model, King, R. B.; Silaghi-Dumitrescu, I, *Dalton Transactions* (2008), (44), 6083-6088.

When Arsine Makes the Difference: Chelating Phosphino and Bridging Arsinioarythiolato Gallium, Valean, Ana Maria; Gomez-Ruiz, Santiago; Lonnecké, Peter; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Hey-Hawkins, Evamarie, *Inorganic Chemistry* (2008), 47(23), 11284-11293.

1,1,4,4-Tetrabenzyl-1,4-diphosphinane-1,4-dium dibromide deuteriochloroform disolvate, Fild, Manfred; Krueger, Oana N.; Silaghi-Dumitrescu, Ioan; Thoene, Carsten, *Acta Crystallographica, Section E: Structure Reports Online* (2007), E63(12), o4525, o4525/1-o4525/8.

1,3-Digermacyclobutanes with exocyclic C:P and C:P:S double bonds. Petrar, Petronela Maria; Nemes, Gabriela; Silaghi-Dumitrescu, Ioan; Ranaivonjatovo, Henri; Gornitzka, Heinz; Escudie, Jean, *Chemical Communications* (2007), (40), 4149-4151

Calix[n]arene derivatives with binding properties toward Eu³⁺, Saponar, Alina; Silaghi-Dumitrescu, Ioan; Popovici, Elisabeth-Jeanne; Popovici, Nicolae, *Studia Universitatis Babes-Bolyai, Chemia* (2007), 52(4), 67-74.

Synthesis of Ester Derivatives of Calix[n]arene, Saponar, Alina; Popovici, Elisabeth-Jeanne; Grecu, Rodica; Silaghi-Dumitrescu, Ioan; Popovici, Nicolae, *Studia Universitatis Babes-Bolyai, Chemia* (2009), 54(4), 203-210.

cis- -1,4-Diphenyl-1,4-diphosphorinane- 2P:P'-bis[pentacarbonylchromium(0)] deuteriochloroform solvate, Fild, Manfred; Krueger, Oana N.; Silaghi-Dumitrescu, Ioan; Thoene, Carsten; Weinkauff, Andreas, *Acta Crystallographica, Section E: Structure Reports Online* (2007), E63(12), m3011, m3011/1-m3011/9.

Density functional theory study of twelve-atom germanium clusters: conflict between the Wade-Mingos rules and optimum vertex degrees, King, R. Bruce; Silaghi-Dumitrescu, Ioan; Uta, Matei M, Dalton Transactions (2007), (3), 364-372.

New [4.4]cyclophane diketals, monoketones, and diketones: design, synthesis, and structural analysis, Bogdan, Niculina; Grosu, Ion; Condamine, Eric; Toupet, Loiec; Ramondenc, Yvan; Silaghi-Dumitrescu, Ioan; Ple, Gerard; Bogdan, Elena, European Journal of Organic Chemistry (2007), (28), 4674-4687.

New Digermylalkenes and Digermylalkynes: [1,3]-Chlorine Shifts in Organogermanium Chemistry? Nemes, Gabriela; Escudie, Jean; Silaghi-Dumitrescu, Ioan; Ranaivonjatovo, Henri; Silaghi-Dumitrescu, Luminita; Gornitzka, Heinz, Organometallics (2007), 26(21), 5136-5139.

Secondary interactions in heteroallenic systems with P:C-E units, Nemes, G.; Silaghi-Dumitrescu, I.; Petrar, P. M.; Septelean, R.; Silaghi-Dumitrescu, L, Studia Universitatis Babes-Bolyai, Chemia (2007), 52(1), 3-9.

Silatropic migration in (1-trimethylsilylindenyl)(indenyl)dimethylsilane, bis(1-trimethylsilylindenyl)dimethylsilane and related compounds, Nemes, Gabriela; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Escudie, Jean; Ranaivonjatovo, Henri; Zukerman-Schpector, Julio, Revue Roumaine de Chimie (2007), 52(8-9), 809-816.

Studies on some ozone decomposition catalysts based on nickel oxide, Dan, Crina; Popovici, Elisabeth-Jeanne; Imre, Florica; Indrea, Emil; Marginean, Petre; Silaghi-Dumitrescu, Ioan, Studia Universitatis Babes-Bolyai, Chemia (2007), 52(1), 91-95.

Synthesis and characterization of calix[4]arene with different donor groups at the "narrow" rim, Saponar, Alina; Silaghi-Dumitrescu, Ioan; Popovici, Elisabeth-Jeanne; Popovici, Nicolae, Revista de Chimie (2007), 58(5), 481-483.

Synthesis and characterization of some mixed ligand zinc(II) complexes of theophylline, Mihaly, Bela; Forizs, Edit; Silaghi-Dumitrescu, Ioan, Studia Universitatis Babes-Bolyai, Chemia (2007), 52(4), 111-116.

Synthesis and characterization of the first arsanylbis(methylene)phosphorane (Me₃Si)₂C:P(Mes^{*}):C(Cl)As(F)Mes^{*}, Petrar, Petronela Maria; Nemes, Gabriela; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Escudie, Jean; Gornitzka, Heinz; Ranaivonjatovo, Henri, Revue Roumaine de Chimie (2007), 52(1-2), 45-49.

Synthesis and properties of organogermanium and organotin dithiophosphonate complexes; crystal structures of (C₆H₅)₂Sn(Cl)[(p-MeOC₆H₄)(EtO)PS₂-S, S'], Me₂Sn[(p-MeOC₆H₄)(MeO)PS₂-S]₂, Me₂Sn[(p-MeOC₆H₄)(iPrO)PS₂-S]₂, and Me₂Ge{[(C₆H₅)₃SiO](p-MeOC₆H₄)PS₂-S]₂, Fild, Manfred; Krueger, Oana; Silaghi-Dumitrescu, Ioan; Thoene, Carsten; Weinkauff, Andreas, Phosphorus, Sulfur and Silicon and the Related Elements (2007), 182(10), 2283-2310.

Synthesis and spectral characterization of some calix[4]pyrogallolarenes, Popovici, N.; Ursales, T. N.; Silaghi-Dumitrescu, I.; Saponar, Alina; Popovici, Elisabeth-Jeanne, Acta Universitatis Cibiniensis, Seria F: Chemia (2007), 10(2), 51-57.

IOAN SILAGHI-DUMITRESCU
1950-2009

The formylation of bis-(N-alkyl-phenothiazinyl)-methane; a theoretical approach, Porumb, Dan; Silaghi-Dumitrescu, Ioan; Gaina, Luiza; Silaghi-Dumitrescu, Luminita; Cristea, Castelia; Cormos, Gabriela, *Studia Universitatis Babes-Bolyai, Chemia* (2007), 52(4), 39-42.

Towards new double-bonded organophosphorus derivatives of C:P:C:P type, Nemes, Gabriela; Septelean, Raluca; Petrar, Petronela M.; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan, *Studia Universitatis Babes-Bolyai, Chemia* (2007), 52(4), 89-94.

α -(3,7-Dioxo- α -1-azabicyclo[3.3.0]oct-5-ylmethoxy)-diazines. Part 2: Functionalization via directed ortho-metalation and cross-coupling reactions, Berghian, Camelia; Condamine, Eric; Ple, Nelly; Turck, Alain; Silaghi-Dumitrescu, Ioan; Maieranu, Carmen; Darabantu, Mircea, *Tetrahedron* (2006), 62(31), 7339-7354.

A quantum chemical conformational analysis of p-tert-butyl/pentyl/octyl-calix[8]arenes, Lupan, Alexandru; Saponar, Alina; Silaghi-Dumitrescu, Ioan; Kun, Attila; Silaghi-Dumitrescu, Luminita; Popovici, Elisabeth Jeanne, *Studia Universitatis Babes-Bolyai, Chemia* (2006), 51(2), 27-34.

Butterfly Diradical Intermediates in Photochemical Reactions of Fe₂(CO)₆(μ -S₂), Silaghi-Dumitrescu, Ioan; Bitterwolf, Thomas E.; King, R. Bruce, *Journal of the American Chemical Society* (2006), 128(16), 5342-5343.

Co-complexes of ortho-dilithiated thiophenol or 2-trimethylsilylthiophenol with lithiated TMEDA molecules: synthesis, crystal structures and theoretical studies (TMEDA = N,N,N',N'-tetramethylethylenediamine), Hildebrand, Alexandra; Loennecke, Peter; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Hey-Hawkins, Evamarie, *Dalton Transactions* (2006), (7), 967-974.

Density Functional Theory Study of 10-Atom Germanium Clusters: Effect of Electron Count on Cluster Geometry. King, R. B.; Silaghi-Dumitrescu, I.; Uta, M. M, *Inorganic Chemistry* (2006), 45(13), 4974-4981.

DFT and the electromerism in complexes of iron with diatomic ligands, Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan., *Journal of Inorganic Biochemistry* (2006), 100(1), 161-166.

First synthesis of a G-2 melamine dendrimer with serinolic peripheral groups, Darabantu, Mircea; Pintea, Monica; Fazekas, Marijana; Lameiras, Pedro; Berghian, Camelia; Delhom, Isabelle; Silaghi-Dumitrescu, Ioan; Ple, Nelly; Turck, Alain, *Letters in Organic Chemistry* (2006), 3(12), 905-910.

Molecular Rotors: Design, Synthesis, Structural Analysis, and Silver Complex of New [7.7]Cyclophanes, Bogdan, Niculina; Grosu, Ion; Benoit, Guillaume; Toupet, Loiec; Ramondenc, Yvan; Condamine, Eric; Silaghi-Dumitrescu, Ioan; Ple, Gerard, *Organic Letters* (2006), 8(12), 2619-2622.

New halo compounds of silicon and tin, potential precursors of >E=C=P-heteroallenic systems, Petrar, Petronela Maria; Nemes, Gabriela; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita, *Studia Universitatis Babes-Bolyai, Chemia* (2006), 51(1), 77-82

IOAN SILAGHI-DUMITRESCU
1950-2009

New low symmetry low energy structures of 11-atom bare germanium clusters: A density functional theory study, King, R. B.; Silaghi-Dumitrescu, I.; Lupan, A, *Chemical Physics* (2006), 327(2-3), 344-350.

Phosphavinylidene(oxo)phosphorane Mes*P(O):C:PMes*: a diphosphaallene featuring λ 5 σ 3- and λ 3 σ 2-phosphorus atoms, Septelean, Raluca; Ranaivonjatovo, Henri; Nemes, Gabriela; Escudie, Jean; Silaghi-Dumitrescu, Ioan; Gornitzka, Heinz; Silaghi-Dumitrescu, Luminita; Massou, Stephane, *European Journal of Inorganic Chemistry* (2006), (21), 4237-4241.

Special issue: Computational inorganic chemistry - Part 3 of 3. [In: Chemtracts; 2006, 19(2)], Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan. USA. (2006), 41 pp. Publisher: (Data Trace Publishing Co., Baltimore, Md.) Book written in English. CAN 146:175448 AN 2007:

Special theme issue inorganic computational chemistry, Part I. [In: Chemtracts, 2006; 18(11)], Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan; Editors. USA. (2006), 41 pp. Publisher: (Data Trace Publishing Co., Baltimore, Md.) Book written in English. CAN 146:175447 AN 2006:1324965

Structural, energetic and electronic characterization of the chiral carbon-nitride nanotubes, Rada, Simona; Silaghi-Dumitrescu, Ioan, *Revue Roumaine de Chimie* (2006), 51(2), 141-145.

Synthesis of new bromo-stannanes: toward unsaturated tin derivatives, Petrar, Petronela Maria; Nemes, Gabriela; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita, *Studia Universitatis Babeş-Bolyai, Chemia* (2006), 51(2), 35-40.

A quantum chemical study on boron nitride and carbon nitride nanotubes., Rada, Simona; Dumitrescu, Ioan Silaghi, *Studia Universitatis Babeş-Bolyai, Chemia* (2005), 50(2), 155-158.

A surprisingly stable 1-(chlorosilyl)-2-phosphaethenyllithium compound, RCl₂SiC(Li):PMes*, Nemes, Gabriela Cretiu; Ranaivonjatovo, Henri; Escudie, Jean; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Gornitzka, Heinz, *European Journal of Inorganic Chemistry* (2005), (6), 1109-1113.

Adsorption of 6-mercaptopurine and 6-mercaptopurine riboside on silver colloid: a pH dependent surface enhanced Raman spectroscopy and density functional theory study. Part I. 6-Mercaptopurine, Szeghalmi, A. V.; Leopold, L.; Pinzaru, S.; Chis, V.; Silaghi-Dumitrescu, I.; Schmitt, M.; Popp, J.; Kiefer, W, *Journal of Molecular Structure* (2005), 735-736 103-113.

Anodic oxidation of difluorenyls bridged through a dimethylsilyl group and of the 9-trimethylsilyl fluorene: Towards new three-dimensional polyfluorenes, Silaghi-Dumitrescu, Ioan; Escudie, Jean; Cretiu-Nemes, Gabriela; Raoult, Eugene; Rault-Berthelot, Joelle, *Synthetic Metals* (2005), 151(2), 114-119

Applications of carbon-nitride nanotubes to molecular engines photochemically engineered, Rada, Simona; Dumitrescu, Ioan Silaghi; Maties, Vistrian; Rada, Marius, *Revista de Chimie (Bucharest, Romania)* (2005), 56(5), 490-494.

IOAN SILAGHI-DUMITRESCU
1950-2009

Computational inorganic chemistry - a useful tool and more, Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan, *Chemtracts* (2005), 18(11), 595-619.

Density Functional Study of 8- and 11-Vertex Polyhedral Borane Structures: Comparison with Bare Germanium Clusters, King, R. B.; Silaghi-Dumitrescu, I.; Lupan, A, *Inorganic Chemistry* (2005), 44(22), 7819-7824.

Density Functional Theory Study of 11-Atom Germanium Clusters: Effect of Electron Count on Cluster Geometry, King, R. B.; Silaghi-Dumitrescu, I.; Lupan, A, *Inorganic Chemistry* (2005), 44(10), 3579-3588.

Density functional theory study of eight-atom germanium clusters: effect of electron count on cluster geometry, King, R. B.; Silaghi-Dumitrescu, I.; Lupan, A, *Dalton Transactions* (2005), (10), 1858-1864

Difluorenylsilanes, -germanes, and -stannanes Exhibiting an Unprecedented Parallel Arrangement of the Fluorene Units, Nemes, Gabriela Cretiu; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Escudie, Jean; Ranaivonjatovo, Henri; Molloy, Kieran C.; Mahon, Mary F.; Zukerman-Schpector, Julio, *Organometallics* (2005), 24(6), 1134-1144.

Discontinuum between ferrous-superoxo and ferric-peroxo in heme [FeO₂]⁹ complexes? Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan, *Studia Universitatis Babes-Bolyai, Chemia* (2005), 50(1), 11-15.

Electronic properties of C₈₀-xN_x tubes with chair geometry, Rada, Simona; Dumitrescu, Ioan Silaghi; Maties, Vistrian; Rada, Marius, *Revista de Chimie* (2005), 56(2), 144-147.

Germanium cluster polyhedra: a density functional theory study, Silaghi-Dumitrescu, Ioan; Kun, Attila; Lupan, Alex; King, R. Bruce, *Lecture Series on Computer and Computational Sciences* (2005), 4 A(Advances in Computational Methods in Sciences and Engineering), 804-806. Publisher: Brill Academic Publishers, ISSN: 1573-4196.

Periodic Cages, Diudea, Mircea V.; Nagy, Csaba L.; Silaghi-Dumitrescu, Ioan; Graovac, Ante; Janezic, Dusanka; Vikić-Topić, Drazen, *Journal of Chemical Information and Modeling* (2005), 45(2), 293-299

75. Structural, energetic and electronic properties of pure/doped BN nanotubes, Rada, Simona; Dumitrescu, Ioan Silaghi, *Studia Universitatis Babes-Bolyai, Chemia* (2005), 50(1), 297-306.

Synthesis and Stereochemistry of New Bis(1,3-Oxathian-2-yl) Derivatives: Epimerisation and Chair-Twist Equilibria, Cismas, C.; Grosu, I.; Ple, G.; Condamine, E.; Ramondenc, Y.; Toupet, L.; Silaghi-Dumitrescu, I.; Nemes, G.; Terec, A.; Muntean, L *Structural Chemistry* (2005), 16(4), 369-377.

The first evidence for a transient stibaallene ArSbCCR₂, Baiget, Lise; Ranaivonjatovo, Henri; Escudie, Jean; Nemes, Gabriela Cretiu; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita, *Journal of Organometallic Chemistry* (2005), 690(2), 307-312.

IOAN SILAGHI-DUMITRESCU
1950-2009

The shapes of hypoelectronic six-vertex anionic bare boron clusters: effects of the countercations, King, R. B.; Silaghi-Dumitrescu, I.; Lupan, A.; Kun, A, *Main Group Chemistry* (2005), 4(4), 291-302

3,7-dioxa-1-azabicyclo[3.3.0]octanes substituted at the C-5 position - >From local to global stereochemistry, Darabantu, Mircea; Maiereanu, Carmen; Silaghi-Dumitrescu, Ioan; Toupet, Loic; Condamine, Eric; Ramondenc, Yvan; Berghian, Camelia; Ple, Gerard; Ple, Nelly, *European Journal of Organic Chemistry* (2004), (12), 2644-2661.

A complex problem of diastereoisomerism: Synthesis and stereochemistry of 1,4-bis-{r-1-aza-c-5-ethyl-3,7-dioxabicyclo[3.3.0]octane-c-2-yl}-benzene, Maiereanu, Carmen; Toupet, Loic; Condamine, Eric; Silaghi-Dumitrescu, Ioan; Ple, Gerard; Ramondenc, Yvan; Darabantu, Mircea, *Revue Roumaine de Chimie* (2004), 49(7), 595-602.

A novel disiloxanediolato-derivative of tin(IV), Petrar, Petronela M.; Nemes, Gabriela Cretiu; Silaghi-Dumitrescu, Ioan. *Studia Universitatis Babes-Bolyai, Chemia* (2004), 49(2), 209-216.

Conformational and configurational analysis on some calix[4]resorcinarenes functionalized with organo-phosphorus groups, Ursales, Traian-Nicolae; Silaghi-Dumitrescu, Ioan, *Revue Roumaine de Chimie* (2004), 49(2), 143-147.

Electronic properties of the zigzag carbon-nitride nanotubes, Rada, Simona; Dumitrescu, Ioan Silaghi. *Studia Universitatis Babes-Bolyai, Chemia* (2004), 49(2), 217-222.

Hemes revisited by density functional approaches. 1: The axial ligand and the dioxygen-peroxo chemistry, Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan *Revue Roumaine de Chimie* (2004), 49(3-4), 257-268.

New materials based on phosphorylated calix[n]arenes, Ursales, T. N.; Silaghi-Dumitrescu, I.; Popovici, E.-J.; Ursales, A.; Popovici, N *Journal of Optoelectronics and Advanced Materials* (2004), 6(1), 307-313.

Possible hybrids between polyoxometalates and calixarenes, Ursales, T. N.; Silaghi-Dumitrescu, I.; Grecu, R.; Silaghi-Dumitrescu, L.; Popovici, N.; Popovici, E.-J, *Journal of Optoelectronics and Advanced Materials* (2004), 6(2), 471-476.

Synthesis of calix[n]arenes with pendant diphenyl phosphate functionalities at the "narrow rim", Ursales, T.-N.; Popovici, N.; Silaghi-Dumitrescu, I.; Popovici, E.-J, *Acta Universitatis Cibiniensis, Seria F: Chemia* (2004), 7(1), 71-75.

Synthesis of some new O-alkenyl calix[6]arene and calix[8]arene derivatives, Ursales, Traian-Nicolae; Silaghi-Dumitrescu, Ioan; Ciocan, Cristina; Palibroda, Nicolae; Popovici, Nicolae; Popovici, Elisabeth-Jeanne. *Revue Roumaine de Chimie* (2004), 49(9), 741-745.

The conformational analysis of some calix[4]arenes substituted at the "lower rim" with organo-phosphorus groups, Ursales, Traian-Nicolae; Silaghi-Dumitrescu, Ioan, *Revue Roumaine de Chimie* (2004), 49(5), 437-441.

Tin(IV) halide complexes of AsPh₃) The structures of trans-SnCl₄(AsPh₃)₂ and SnBr₄(AsPh₃)₂, Mahon Mary F; Moldovan Natalia L; Molloy Kieran C; Muresan Alexandra; Silaghi-Dumitrescu Ioan; Silaghi-Dumitrescu Luminita, *Dalton transactions* (2004), (23), 4017-21.

1-Aza-5-hydroxymethyl-3,7-dioxabicyclo[3.3.0]octanes: Chelating properties related to their conformational chirality, Maieranu, Carmen; Condamine, Eric; Silaghi-Dumitrescu, Ioan; Darabantu, Mircea, *Studia Universitatis Babes-Bolyai, Chemia* (2003), 48(2), 91-101.

Azocoupling products. Part IV. The structure of dyes obtained by azo-coupling reaction of 1-(4-hydroxy-6-methylpyrimidin-2-yl)-3-methylpyrazolin-5-one with aromatic diazonium salts, Panea, Ioan; Ghirisan, Adina; Baldea, Ioan; Silaghi-Dumitrescu, Ioan; Craciun, Liliana; Silberg, Ioan A, *Studia Universitatis Babes-Bolyai, Chemia* (2003), 48(2), 67-83.

Computational Study of the Non-Heme Iron Active Site in Superoxide Reductase and Its Reaction with Superoxide, Silaghi-Dumitrescu, Radu; Silaghi-Dumitrescu, Ioan; Coulter, Eric D.; Kurtz, Donald M., Jr. *Inorganic Chemistry* (2003), 42(2), 446-456

Computational study of the non-heme iron active site in superoxide reductase and its reaction with superoxide, Silaghi-Dumitrescu Radu; Silaghi-Dumitrescu Ioan; Coulter Eric D; Kurtz Donald M Jr, *Inorganic chemistry* (2003), 42(2), 446-56.

Density Functional Theory Study of Nine-Atom Germanium Clusters: Effect of Electron Count on Cluster Geometry, King, R. B.; Silaghi-Dumitrescu, I, *Inorganic Chemistry* (2003), 42(21), 6701-6708.

Density functional theory study of nine-atom germanium clusters: effect of electron count on cluster geometry, King R B; Silaghi-Dumitrescu I, *Inorganic chemistry* (2003), 42(21), 6701-8.

Influences of Changes in Multitopic Tris(pyrazolyl)methane Ligand Topology on Silver(I) Supramolecular Structures, Reger, Daniel L.; Semeniuc, Radu F.; Silaghi-Dumitrescu, Ioan; Smith, Mark D *Inorganic Chemistry* (2003), 42(12), 3751-3764.

Influences of changes in multitopic tris(pyrazolyl)methane ligand topology on silver(I) supramolecular structures, Reger Daniel L; Semeniuc Radu F; Silaghi-Dumitrescu Ioan; Smith Mark D, *Inorganic chemistry* (2003), 42(12), 3751-64

Molecular structure and infrared spectra of 2-bromopropane by ab initio HF and post HF calculations, Grecu, Rodica; Kun, Attila; Silaghi-Dumitrescu, Ioan, *Revue Roumaine de Chimie* (2003), Volume Date 2002, 47(10-11), 1055-1061.

New halo compounds of Si, P, As, and Sb bearing a bulky substituted fluorenyl group, Baiget, L.; Bouslikhane, M.; Escudie, J.; Nemes, G. Cretiu; Silaghi-Dumitrescu, I.; Silaghi-Dumitrescu, L, *Phosphorus, Sulfur and Silicon and the Related Elements* (2003), 178(9), 1949-1961.

IOAN SILAGHI-DUMITRESCU
1950-2009

One pot synthesis a new calix[n]arene derivatives, Ursales, T.-N.; Popovici, E.-J.; Silaghi-Dumitrescu, I.; Popovici, N, Acta Universitatis Cibiniensis, Seria F: Chemia (2003), 6(2), 9-13

Relative stability of conformers of some organophosphorus calix[4]arenes, Ursales, Traian-Nicolae; Silaghi-Dumitrescu, Ioan, Revista de Chimie, (2003), 54(9), 756-758

Small fullerenes, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan, Studia Universitatis Babes-Bolyai, Chemia (2003), 48(1), 21-30.

Stereocontrolled synthesis by anomeric effects of substituted 1-aza-3,7-dioxabicyclo[3.3.0]octanes, Maieranu, Carmen; Silaghi-Dumitrescu, Ioan; Berghian, Camelia; Pinteau, Monica; Fazekas, Marijana; Darabantu, Mircea, Studia Universitatis Babes-Bolyai, Chemia (2003), 48(2), 103-112.

Synthesis and characterization of some new phosphorylated cavitands from calix[4]resorcinarenes, Ursales, Traian-Nicolae; Silaghi-Dumitrescu, Ioan, Revista de Chimie, (2003), 54(11), 888-889.

Synthesis and reactivity of difluoromethylene bridged diphospha-derivatives, Toetes, R.; Silaghi-Dumitrescu, I, Studia Universitatis Babes-Bolyai, Chemia (2003), 48(2), 149-163.

Synthesis, characterization and conformational analysis of methyl-, propyl-, and isopropylcalix[4]resorcinarenes, Ursales, Traian-Nicolae; Ursales, Adina; Silaghi-Dumitrescu, Ioan. Revista de Chimie) (2003), 54(3), 229-231.

A density functional theory study of five-, six- and seven-atom germanium clusters: distortions from ideal bipyramidal deltahedra in hypoelectronic structures, King, R. B.; Silaghi-Dumitrescu, I.; Kun, A, Journal of the Chemical Society, Dalton Transactions (2002), (21), 3999-4004.

Ring-chain tautomerism and other versatile behaviour of 1,4-diimino- and 1,2-phenylene derivatives of some C-substituted serinols. Maieranu, Carmen; Darabantu, Mircea; Ple, Gerard; Berghian, Camelia; Condamine, Eric; Ramondenc, Yvan; Silaghi-Dumitrescu, Ioan; Mager, Sorin. Tetrahedron (2002), 58(13), 2681-2693

Crystal, molecular, and electronic structure of 9,9'-bis(trimethylsilyl)fluorene, Silaghi-Dumitrescu, Ioan; Cretiu, Gabriela; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel; Toscano, Alfredo; Cea-Olivares, Raymundo, Revue Roumaine de Chimie 2001, 46(4), 289-295.

Crystal, molecular, and electronic structure of 9,9'-bis(trimethylsilyl)fluorene, Silaghi-Dumitrescu, Ioan; Cretiu, Gabriela; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel; Toscano, Alfredo; Cea-Olivares, Raymundo, Revue Roumaine de Chimie (2002), 46(4), 289-295.

Difluorenylsilane derivatives, a class of compounds exhibiting strong intra- and intermolecular C-H... π interactions. Crystal and molecular structures of bis(9-methylfluoren-9-yl)dimethylsilane and (9-methylfluoren-9-yl)(fluoren-9-yl)dimethylsilane, Cretiu, Gabriela; Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Escudie, Jean; Toscano, Alfredo; Hernandez, Simon; Cea-Olivares, Raymundo, Journal of Organometallic Chemistry (2002), 659(1-2), 95-101.

IOAN SILAGHI-DUMITRESCU
1950-2009

Electronic structure of hypervalent organoarsenic bromo derivatives. An ab initio RHF and DFT-B3LYP investigation of H5-XAsBr_x systems, Silaghi-Dumitrescu, L.; Silaghi-Dumitrescu, I, *Studia Universitatis Babes-Bolyai, Chemia* (2002), 47(1-2), 203-211.

Toroidal fullerenes from squared tiled tori, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan; Parv, Bazil, *Internet Electronic Journal of Molecular Design* [online computer file] (2002), 1(1), 10-22.

Toroidal fullerenes from squared tiled tori, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan; Parv, Bazil. *Internet Electronic Journal of Molecular Design* [online computer file] (2002), 1(1), 10-22

Distortions from octahedral symmetry in hypoelectronic six-vertex polyhedral clusters of the group 13 elements boron, indium, and thallium as studied by density functional theory, King, R. Bruce; Silaghi-Dumitrescu, Ioan; Kun, Attila, *Inorganic chemistry* (2001), 40(10), 2450-2.

Electronic and magnetic properties of (tetrakis(2-pyridylmethyl)-ethylenediamine)iron(II) perchlorate. A comparison of different computational methods, Chen, Guangju; Liu, Ruozhuang; Silaghi-Dumitrescu, I.; Espinosa-Perez, G.; Zentella-Dehesa, A.; Lara-Ochoa, F, *International Journal of Quantum Chemistry* (2001), 83(2), 60-69.

Solvent effects in infrared spectra and ab initio calculations of 2-bromopropane, Grecu, R.; Kun, A.; Silaghi-Dumitrescu, I, *Journal of Molecular Structure* (2001), 565-566 39-42

Structural distortions in homoleptic (RE)4A (E = O, S, Se; A = C, Si, Ge, Sn): implications for the CVD of tin sulfides, Barone, Giampaolo; Hibbert, Thomas G.; Mahon, Mary F.; Molloy, Kieran C.; Parkin, Ivan P.; Price, Louise S.; Silaghi-Dumitrescu, Ioan, *Journal of the Chemical Society, Dalton Transactions* (2001), (23), 3435-3445.

Toranes versus torenes, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan; Parv, Bazil, *MATCH* (2001), 44 117-133.

Voltammetric behaviour of 1,4-benzothiazino[2,3-b]phenothiazine and some of its derivatives. II. The influence of N-substitution and S-oxidation, Cristea, Castelia; Filip, Cecilia; Silaghi-Dumitrescu, Ioan; Silberg, Ioan A, *Revue Roumaine de Chimie* (2001), 45(7-8), 639-642.

(Tetrakis(2-pyridylmethyl)ethylenediamine)iron(II) Perchlorate. Study of Density Functional Methods, Chen, Guangju; Espinosa-Perez, G.; Zentella-Dehesa, A.; Silaghi-Dumitrescu, I.; Lara-Ochoa, F, *Inorganic Chemistry* (2000), 39(16), 3440-3448.

(Tetrakis(2-pyridylmethyl)ethylenediamine)iron(II) perchlorate. Study of density functional methods, Chen G; Espinosa-Perez G; Zentella-Dehesa A; Silaghi-Dumitrescu I; Lara-Ochoa F, *Inorganic chemistry* (2000), 39(16), 3440-8.

A new tubular arrangement of a dimethylsilyl bridged calix[4]resorcinarene, Lara-Ochoa, F.; Garcia, M. Martinez; Teran, R.; Cruz-Almanza, R.; Espinosa-Perez, G.; Chen, G.; Silaghi-Dumitrescu, I, *Supramolecular Chemistry* (2000), 11(4), 263-273.

IOAN SILAGHI-DUMITRESCU
1950-2009

Bromination of (AsPh₂)₂O: the structure of tribromo-diphenylarsenic(V), Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Radu; Haiduc, Ionel; Blake, Alexander J.; Sowerby, D. Bryan. *Revista de la Sociedad Quimica de Mexico* (2000), 44(2), 134-138.

Synthesis and stereochemistry of some new spiro-1,3-perhydrooxazines, Muntean, Luminita; Grosu, Ion; Ple, Gerard; Mager, Sorin; Silaghi-Dumitrescu, Ioan, *Monatshefte fuer Chemie* (2000), 131(9), 975-983.

Synthesis and stereochemistry of some 1,3-oxazolidine systems based on TRIS (α, α, α -trimethylolaminomethane) and related aminopolyols skeleton. Part 2: 1-aza-3,7-dioxabicyclo[3.3.0]octanes. Darabantu, Mircea; Ple, Gerard; Maieranu, Carmen; Silaghi-Dumitrescu, Ion; Ramondenc, Yvan; Mager, Sorin. *Tetrahedron* (2000), 56(23), 3799-3816

Synthesis and stereochemistry of some 1,3-oxazolidine systems based on TRIS (α, α, α -trimethylolaminomethane) and related aminopolyols skeleton. Part 1: (Di)spiro-1,3-oxazolidines. Darabantu, Mircea; Ple, Gerard; Silaghi-Dumitrescu, Ion; Maieranu, Carmen; Tuross, Istvan; Silberg, Ioan A.; Mager, Sorin. *Tetrahedron* (2000), 56(23), 3785-3798

Is the trigonal prismatic distortion the answer for the geometry of In(III) four members dithiochelate compounds? The crystal and molecular structure of In(S₂AsR₂)₃ (R = Me, Ph). Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ion; Haiduc, Ionel; Toscano, Ruben-Alfredo; Garcia-Montalvo, Veronica; Cea-Olivares, Raymundo. *Zeitschrift fuer Anorganische und Allgemeine Chemie* (1999), 625(2), 347-351

The crystal and molecular structure of the 2,4,6,8-tetra-t-Bu-phenothiazine 0.5 benzene adduct, Silaghi-Dumitrescu, I.; Silberg, I. A.; Filip, S.; Vlassa, M.; Silaghi-Dumitrescu, L.; Hernandez-Ortega, S, *Journal of Molecular Structure* (2000), 526 279-286.

An interactive workstation for molecular-mechanics modeling of chemical structures. Horvat, Dragos; Silaghi-Dumitrescu, Ion. *Revue Roumaine de Chimie* (1992), 37(10), 1165-74

1-(Acridin-9'-yl)-pyrazolin-3- and -5-ones. A new class of heterocycles with potential biological activity, Cristea, Ioan; Popovici, Mariana M.; Mendel, Maria T.; Silaghi-Dumitrescu, Ioan; Kozma, Erika, *Heterocyclic Communications* (1999), 5(6), 543-548.

A new organodithiophosphoric derivative; synthesis and structural characterization of bis(diphenylborano)dithiophosphoric [(C₆H₅)₂BO]₂P(S)SH, Gabriela, Cretiu; Reka, Torok; Delia, Bugnariu; Oxana, Jeman; Silaghi-Dumitrescu, Ioan, *Studia Universitatis Babes-Bolyai, Chemia* (1999), 44(1-2), 177-182.

An AM1 investigation of the structures of C₆₀:tBu-calix[8]arene 1:1 adducts, Lara-Ochoa, F.; Cogordan, J. A.; Cruz, R.; Martinez, M.; Silaghi-Dumitrescu, I, *Fullerene Science and Technology* (1999), 7(3), 411-419.

IOAN SILAGHI-DUMITRESCU
1950-2009

Molecular orbital calculations and physical properties of 1,4-benzothiazino[2,3-b]phenothiazine and its substituted derivatives, Silberg, I. A.; Silaghi-Dumitrescu, I.; Cristea, C.; Tordo, P.; Gignes, D, *Heterocyclic Communications* (1999), 5(2), 147-150.

Stable isomers of sila- and germadodecahedrane. A semiempirical (AM1) investigation of the structure of 4/6 and 4/5/6 ring containing E20 (E=Si,Ge) systems, Silaghi-Dumitrescu, Ioan; Kun, Attila; Haiduc, Ionel, *Fullerene Science and Technology* (1999), 7(5), 841-854.

Why does the yellow isomer of [Sn{(PPh₂Se)₂-Se,Se'}₂] present a square planar four-co-ordinated tin(II)? A molecular orbital approach, Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Cea-Olivares, Raymundo, *Main Group Metal Chemistry* (1999), 22(1), 5-8.

Synthesis and ring-ring tautomerism of some spirooxazolidines based on i-p-nitrophenylserinol skeleton. Darabantu, Mircea; Ple, Gerard; Gaina, Luiza; Maierean, Carmen; Silaghi-Dumitrescu, Ion. *Studia Universitatis Babes-Bolyai, Chemia* (1998), 43(1-2), 179-192

Cis and/or trans dioxaphosphetanes. A molecular orbital study of some model (RPO)₂ systems, Silaghi-Dumitrescu, Ioan; Horea, Alin, *Revue Roumaine de Chimie* (1997), 42(7), 599-604.

Comparative PM3-MO study of the E2O2 and E2N2 (E = P, As) four-membered-ring systems, Silaghi-Dumitrescu, Ioan; Horea, Alin; Pascu, Sofia; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel, *Phosphorus, Sulfur and Silicon and the Related Elements* (1997), 124 & 125 441-444.

Ion-molecule interactions in organic electrochemical systems. I. NMR investigations of electrolyte solutions used in lithium anode batteries, Silberg, Ioan Alexandru; Oniciu, Liviu; Bobos, Liviu-Dorel; Silaghi-Dumitrescu, Ioan; Avram, Silvia; Cuiibus, Cristina. *Revue Roumaine de Chimie* (1997), 42(7), 535-542.

On the formation of cyclodisilazanes via the coordination of bis(dialkylamino)silanes to halosilanes: an ab initio and AM1 molecular orbital study of the 4644 R₂Si(NR'₂)₂:SiX₄ ring systems, Silaghi-Dumitrescu, Ioan; Lara-Ochoa, Francisco; Haiduc, Ionel, *THEOCHEM* (1997), 397 213-222.

On the structure of bis(9-fluorenyl)dimethylsilane: a sterically crowded molecule with relatively low barriers of rotations around the Si-C(fluorenyl) bonds X-ray diffraction analysis and AM1 molecular orbital calculations, Silaghi-Dumitrescu, Luminita; Haiduc, Ionel; Cea-Olivares, Raymundo; Silaghi-Dumitrescu, Ioan; Escudie, Jean; Couret, Claude, *Journal of Organometallic Chemistry* (1997), 545-546 1-7.

Structural studies of tetrazoles. Crystal and molecular structure and ab initio calculations of 1-phenyl-1H-tetrazole-5-thiolate, as its [diaqua(18-crown-6)sodium] salt: an anionic tetrazole free of direct metal interactions, Jimenez-Sandoval, Omar; Cea-Olivares, Raymundo; Hernandez-Ortega, Simon; Silaghi-Dumitrescu, Ioan, *Heteroatom Chemistry* (1997), 8(4), 351-359.

IOAN SILAGHI-DUMITRESCU
1950-2009

The first oxygen-bridged diorganoarsenic(V) compound: the crystal structure of $\text{AsMe}_2(\text{S})\text{OAs}(\text{S})\text{Me}_2$, Silaghi-Dumitrescu, Luminita; Pascu, Sofia; Silaghi-Dumitrescu, Ioan; Haiduc, Ionel; Gibbons, Martin N.; Sowerby, D. Bryan, *Journal of Organometallic Chemistry* (1997), 549(1-2), 187-192.

$\text{A}_{12}\text{B}_{12}$ (A = B,Al; B = N,P) 4/6 fullerene-like cages and their hydrogenated forms stabilized by exohedral bonds. An AM1 molecular orbital study, Silaghi-Dumitrescu, Ioan; Lara-Ochoa, Francisco; Haiduc, Ionel, *THEOCHEM* (1996), 370(1), 17-23.

Coordinative dimerization of aminosilanes. Model MNDO and ab initio molecular orbital calculations, Lara-Ochoa, Francisco; Silaghi-Dumitrescu, Ioan; Haiduc, Ionel. *Main Group Chemistry* (1996), 1(4), 387-398.

Interactions between calix[8]arenes and fullerenes. Molecular dynamics and molecular mechanics simulation of the 1:1 and 1:2 complexes, Lara-Ochoa, Francisco; Cogordan, Juan Antonio; Silaghi-Dumitrescu, Ioan *Fullerene Science and Technology* (1996), 4(5), 887-896

Ion molecule interaction in organic electrochemical systems III. Acrylonitrile-quaternary ammonium cations adducts and their possible implications in electrohydrodimerization processes, Silberg, I. A.; Ciomos, Forentina; Silaghi-Dumitrescu, I, *Studia Universitatis Babes-Bolyai, Chemia* (1996), 41(2), 167-172.

More about boron-nitrogen $\text{B}_{12}+3\text{nN}_{12}+3\text{n}$ fullerene-like cages. An ab initio and AM1 investigation of some 4/6 isomers, Silaghi-Dumitrescu, Ioan; Lara-Ochoa, Francisco; Bishof, Peter; Haiduc, Ionel, *THEOCHEM* (1996), 367 47-54.

Oxidation of $(\text{AsPh}_2)_2\text{E}$ (E = O or S); supramolecular hydrogen-bonded self-assembly of an unusual tetranuclear adduct and crystal structure of $[\text{AsPh}_2(\text{O})\text{OH} \cdot \text{AsPh}_2(\text{S})\text{OH}]_2$, Silaghi-Dumitrescu, Luminita; Gibbons, Martin N.; Silaghi-Dumitrescu, Ioan; Zukerman-Schpector, Julio; Haiduc, Ionel; Sowerby, D. Bryan, *Journal of Organometallic Chemistry* (1996), 517(1-2), 101-106.

On the geometries and electronic structures of XH_2SiNH_2 (X = F, Cl, Br) silanes. MNDO molecular orbital calculations, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Studia Universitatis Babes-Bolyai, Chemia* (1995), 40(1-2), 91-98.

An improved first-order optimization of molecular structure taking account of molecular topology, Horvath, Dragos; Silaghi-Dumitrescu, Ioan, *Studia Universitatis Babes-Bolyai, Chemia* (1994), 39(1-2), 15-27.

An old ligand in a new environment: triply bridged O,O'-dimethyldithiophosphate in the organosamarium complex $[(\text{C}_5\text{Me}_5)_2\text{Sm}\{\text{S}_2\text{P}(\text{OMe})_2\}_2]_2$, Rieckhoff, Melanie; Noltemeyer, Mathias; Edelmann, Frank T.; Haiduc, Ionel; Silaghi-Dumitrescu, Ioan, *Journal of Organometallic Chemistry* (1994), 469(1), C22-C23.

Chelating versus bridging coordination of dithiophosphates in copper complexes. An EHMO study, Silaghi-Dumitrescu, Ioan; Serban, Liliana; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel, *Revue Roumaine de Chimie* (1994), 39(12), 1397-405.

IOAN SILAGHI-DUMITRESCU
1950-2009

On the geometry of 1,3-diazadiphosphetidines. The cis-trans isomerism, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, Phosphorus, Sulfur and Silicon and the Related Elements (1994), 91(1-4), 21-36.

ansa-Metallocene derivatives of samarium and ytterbium with soft donor ligands, Edelmann, Frank T.; Rieckhoff, Melanie; Haiduc, Ionel; Silaghi-Dumitrescu, Ioan, Journal of Organometallic Chemistry (1993), 447(2), 203-8.

Fully inorganic (carbon-free) fullerenes? The boron-nitrogen case, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel; Sowerby, D. Bryan, Inorganic Chemistry (1993), 32(17), 3755-8.

On the ring angles in the four-membered cyclodiphosphazanes, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, Studia Universitatis Babes-Bolyai, Chemia (1993), 38(1-2), 183-186.

Molecular topology. 2. A computer program for multiple bond, cycle and radical approximations of DS index, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan, Revue Roumaine de Chimie (1991), 36(1-3), 263-9.

Molecular topology. 2. A computer program for multiple bond, cycle and radical approximations of DS index, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan, Revue Roumaine de Chimie (1991), 36(8), 975-82.

The richness of structures available to P₂N₂ inorganic heterocycles. A topological and molecular orbital (EHMO) analysis, Haiduc, Ionel; Silaghi-Dumitrescu, Ioan, Revue Roumaine de Chimie (1991), 36(4-7), 527-44.

The electronic structure of silyl amide ([H₃SiNSiH₃]⁻) anion. A simple molecular orbital treatment, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, Revue Roumaine de Chimie (1990), 35(3), 475-84.

The infrared spectra of methyl(O-methyl)dithiophosphonic acid. Multiplicity of some bands due to different conformers, Grecu, Rodica; Constantinescu, Rodica; Silaghi-Dumitrescu, I.; Haiduc, IJournal of Molecular Structure (1990), 218 111-16.

Molecular structure modeling by using a basic line formula interpreter, Horvath, D.; Silaghi-Dumitrescu, I, Studia Universitatis Babes-Bolyai, Chemia (1989), 34(2), 41-5.

Molecular topology. I. Valence group electronegativity as a vertex discriminator, Diudea, Mircea V.; Silaghi-Dumitrescu, Ioan Revue Roumaine de Chimie (1989), 34(5), 1175-82.

The sulfotropic molecular rearrangement of tetraorganodiarsine disulfides, Silaghi-Dumitrescu, Luminita; Silaghi-Dumitrescu, Ioan; Haiduc, Ionel. Revue Roumaine de Chimie (1989), 34(1), 305-15.

Vibrational spectra and coordination behavior of organo-dithiophosphorus ligands, Silaghi-Dumitrescu, Ioan; Grecu, Rodica; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel, Studia Universitatis Babes-Bolyai, Chemia (1989), 34(1), 97-101.

IOAN SILAGHI-DUMITRESCU
1950-2009

Electronic structure and bonding in diamidoboron cations. A molecular orbital study of diamidoboron(1+) [H₂NBNH₂]⁺, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Revue Roumaine de Chimie* (1988), 33(9-10), 851-6.

Linear versus bent bis(diphosphine)iminium cations. A molecular orbital discussion of the bonding in [H₃PNPH₃]⁺ and related species, Silaghi-Dumitrescu, I.; Haiduc, I, *Revue Roumaine de Chimie* (1988), 33(2), 133-42.

Inorganic (carbon-free) chelate rings, Haiduc, Ionel; Silaghi-Dumitrescu, Ioan *Coordination Chemistry Reviews* (1986), 74 127-270.

The bonding in dialkyldithiophosphinato metal complexes. A molecular orbital study of bis(dimethyldithiophosphinato)nickel(II), Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Revue Roumaine de Chimie* (1986), 31(11-12), 955-62.

Why are cyclodisilazane rings more stable than cyclodisiloxanes? A qualitative molecular orbital approach to the bonding in cyclodisilazanes and cyclodisiloxanes, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Inorganica Chimica Acta* (1986), 112(2), 159-65.

The crystal and molecular structure of a versatile bidentate ligand: tetraphenyldithioimidodiphosphinate, Ph₂(S)PNHP(S)Ph₂, Hitchcock, Peter B.; Nixon, John F.; Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Inorganica Chimica Acta* (1985), 96(1), 77-80.

The electronic structure and bonding in the thiophosphoryl cation PS⁺, Silaghi-Dumitrescu, I.; Haiduc, I, *Phosphorus and Sulfur and the Related Elements* (1985), 22(1), 85-91.

Electronic structure and force constants of the dithionitronium cation NS₂⁻, Silaghi-Dumitrescu, I.; Haiduc, I, *THEOCHEM* (1984), 15(3-4), 217-23.

Vibrational spectra of phosphorodithioic metal complexes. Normal coordinate treatment of bis(O-isopropyl ethyldithiophosphonato)nickel(II), Haiduc, I.; Silaghi-Dumitrescu, I.; Grecu, Rodica; Constantinescu, Rodica; Silaghi-Dumitrescu, Luminita, *Journal of Molecular Structure* (1984), 114 467-70.

Bonding in organophosphorus dithio acids. A CNDO/2 calculation of electronic structure, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, *Phosphorus and Sulfur and the Related Elements* (1982), 12(2), 205-12.

Normal coordinate analysis of the vibrational spectrum of dimethyldithioarsinato anion, (CH₃)₂AsS₂⁻, Silaghi-Dumitrescu, Ioan; Silaghi-Dumitrescu, Luminita; Haiduc, Ionel, *Revue Roumaine de Chimie* (1982), 27(8), 911-16.

A simple topology-based method for estimating stretching force constants of AB_n molecules, Silaghi-Dumitrescu, I *Revue Roumaine de Chimie* (1981), 26(11-12), 1441-5.

IOAN SILAGHI-DUMITRESCU
1950-2009

The infrared spectrum of dimethyldithiophosphinato anion (CH₃)₂ PS₂⁻. Normal coordinate analysis and Urey-Bradley force field calculation, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel, Revue Roumaine de Chimie (1980), 25(6), 815-21.

Vibrational characteristics of nickel(II) dithiophosphinato chelates. Normal coordinate analysis and Urey-Bradley force field calculation of Ni[S₂P(CH₃)₂]₂, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel Revue Roumaine de Chimie (1980), 25(6), 823-30.