



IOAN SILAGHI-DUMITRESCU
1950-2009

Corresponding member of the Romanian Academy

Born in 1950, he attended primary school in his home village (Botiz, Satu Mare county) and followed on with highschool in Satu-Mare.

Graduated in 1974 from the Inorganic Chemistry of the Department of Chemistry of the Babes-Bolyai University at Cluj-Napoca, Romania, he obtained his PhD from the same university in 1981. After three years spent in the industry at the Sanex Enterprise for Fine Ceramics in Construction (1974-1977), he joined the faculty at the Department of Chemistry and Chemical Engineering of the Babes-Bolyai University, where he eventually became a full professor in 1994; here, he served as head of the Inorganic Chemistry Chair (1994-2007) and as Dean of the Department (2008-2009).

Professor Ioan Silaghi-Dumitrescu's research contributions were in the fields of inorganic and organometallic chemistry, with synthesis and structural characterization of transition metal compounds as well as of compounds involving elements from main groups 13, 14 and 15 (e.g., cumulene and heterocumulene systems with heavy elements, biologically-active compounds).

IOAN SILAGHI-DUMITRESCU
1950-2009

He was among the first researchers in Romania to approach chemistry with computational techniques, starting very early on from force constant calculations and spectrum simulations to offer general principles for assigning coordination modes with thiophosphoric ligands at a time when structural analysis with X-ray diffraction was not available in Romania. He then evolved towards quantum chemistry, where he provided notable contributions with molecular modeling studies. His results on the structure of clusters involving main group (post-transition) elements, organometallic clusters, cumulenic and heterocumulenic systems, nanotubes and calixarenes, were reported in journals among the most prestigious in the field of chemistry. Much of his research was aimed not solely at obtaining structural information, but also at understanding and guiding experiments performed in his own research group as well as by collaborators from various countries, thereby allowing for establishing strategies in synthesis and for explanation and prediction of properties for a wide range of inorganic, organometallic and organic compounds. His results have been reported in 182 scientific articles in relevant journals across the world (December 2009).

The Center for Molecular Modeling and Quantum Chemistry founded by him in 2007 (developed from the Laboratory for Structure and Molecular Modeling established in 1996), featuring an internationally-competitive computational infrastructure, has consolidated the school of theoretical chemistry in Cluj and has provided a sound basis for high-level collaborations with prominent researchers from the United States of America and from China.

He was a visiting professor at the National Autonomous University in Mexico (UNAM) in the Theoretical Chemistry Group at the Institute of Chemistry (1995-1996) and at the University of Georgia, Athens, Georgia (USA) (2000-2008, for 1-2 months each year). He also had research-related stays at the University of Nottingham (1992) and Heidelberg University (1993-1994), and was engaged in active collaborations with groups from the Universities in Toulouse, Rouen, Lille, Leipzig, Braunschweig, Köln, Budapest, Pecs, Beijing, Guanjou, Moskow (Idaho).

He received the "*Gheorghe Spacu*" prize from the Romanian Academy for his "Research in structure and molecular topology" in 1989 and the "*Gheorghe Spacu*" Medal and "Diploma de Onoare" from the Romanian Society of Chemistry (2009).

Editorial Board

Ioan Silaghi-Dumitrescu - List of Publications

Binuclear cyclopentadienylcobalt sulfur and phosphinidene complexes $\text{Cp}_2\text{Co}_2\text{E}_2$ ($\text{E} = \text{S}, \text{PX}$): 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 $\text{Co}_2(\text{CO})_6\text{E}_2$ ($\text{E} = \text{S}, \text{PX}$), 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 cobaltadecaboranes, 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.

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(phosphanyl amino)benzene ligands: a zinc(II) complex and an unusual nickel(I) complex with a Dewar-benzene-type Ni₂P₂N₂ backbone, Majoumo-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.

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, Pintea, 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 Arsinoarylthiolato Gallium, Vanean, Ana Maria; Gomez-Ruiz, Santiago; Lonnecke, 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-diium 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.; Septelea, 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.

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-Dioxa-r-1-azabicyclo[3.3.0]oct-c-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, Loic; 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

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 Babes-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 Babes-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.

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 stiballene 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.

The shapes of hypoelectronic six-vertex anionic bare boron clusters: effects of the counteractions, 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; Maieranu, 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, Maieranu, 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.

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; Pinte, 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, Toetoes, 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.

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.

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; Turos, 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 dithiochelat 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.

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.; Gimes, 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; Maiercan, 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; Cuius, 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.

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.

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, Ionel, Journal 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.

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 $(\text{CH}_3)_2\text{PS}_2^-$. 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 $\text{Ni}[\text{S}_2\text{P}(\text{CH}_3)_2]_2$, Silaghi-Dumitrescu, Ioan; Haiduc, Ionel *Revue Roumaine de Chimie* (1980), 25(6), 823-30.

