



ROMÂNIA
UNIVERSITATEA BABEȘ-BOLYAI CLUJ-NAPOCA

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RECTORATUL

Universitatea Babeș-Bolyai Competiția Excelenței 2010

Dosar individual

Notă: Toate datele se referă la perioada 2005-2009

Nume, prenume, grad did.	SILAGHI_DUMITRESCU IOAN, PROFESOR
Facultatea, Catedra	Facultatea de Chimie si Inginerie Chimica, Catedra de Chimie Anorganica
Domeniul științific	Chimie
Adresa paginii web personale	http://chem.ubbcluj.ro/pagini/anorganica/isi.html
Adresa e-mail	

Criteriaul I – Output

1. Articole științifice publicate în reviste indexate ISI (cu menționare factorului de impact în cazul celor cotate)

1. On the microwave-assisted synthesis of acylphenothiazine derivatives - Experiment versus theory synergism
Gaina, L; Porumb, D; Silaghi-Dumitrescu, I; Cristea, C; Silaghi-Dumitrescu, L
CANADIAN JOURNAL OF CHEMISTRY-REVUE CANADIENNE DE CHIMIE 88 (1):42-49 2010

2. Binuclear cyclopentadienylcobalt sulfur and phosphinidene complexes Cp₂Co₂E₂ (E = S, PX): Comparison with their Iron carbonyl analogues
Li, GL; Li, QS; Silaghi-Dumitrescu, I; King, RB; Schaefer, HF
JOURNAL OF ORGANOMETALLIC CHEMISTRY 695 (6):804-808 2010

3. Endohedral Nickel, Palladium, and Platinum Atoms in 10-Vertex Germanium Clusters: Competition between Bicapped Square Antiprismatic and Pentagonal Prismatic Structures
King, RB; Silaghi-Dumitrescu, I; Uta, AM
JOURNAL OF PHYSICAL CHEMISTRY A 113 (3):527-533 2009

4. vic-Dichlorodiphosphapropenes - Synthesis and Coordination Ability
Septelean, R; Nemes, G; Escudie, J; Silaghi-Dumitrescu, I; Ranaivonjatovo, H; Petrar, P; Gornitzka, H; Silaghi-Dumitrescu, L; Saffon, N
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY (5):628-634 2009

5. N,N' and N,O chelated phosphonium cations containing aminotroponimate or aminotroponate units
Pop, LC; Katir, N; Castel, A; Silaghi-Dumitrescu, L; Delpesch, F; Silaghi-Dumitrescu, I; Gornitzka, H; MacLeod-Carey, D; Saffon, N
JOURNAL OF ORGANOMETALLIC CHEMISTRY 694 (9-10):1562-1566 2009

6. Narrow-Rim Alkenyl Calix[n]Arene Synthesis and Spectral Characterization
Saponar, A; Popovici, EJ; Popovici, N; Bica, E; Nemes, G; Petrar, P; Silaghi-Dumitrescu, I
REVISTA DE CHIMIE 60 (3):278-282 2009

7. (Diethylenetriamine)bis(theophyllinato)zinc(II) dihydrate
Mihaly, B; Forizs, E; Kun, AZ; Silaghi-Dumitrescu, I
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE 65M579-U1038 2009

8. Kinetic versus Thermodynamic Isomers of the Deltahedral Cobaltadiboraboranes
King, RB; Silaghi-Dumitrescu, I; Sovago, I
INORGANIC CHEMISTRY 48 (12):5088-5095 2009
9. An insight into the structure of model germaphosphaallenes
Petrar, PM; Nemes, G; Silaghi-Dumitrescu, I; Escudie, J; Ranaivonjatovo, H
MOLECULAR PHYSICS 107 (8-12):1161-1167 2009
10. Stabilisation of an inorganic digallane by the phosphinobisthiolato P,S,S pincer ligand PPh(2-SC₆H₄)(2)
Valean, AM; Gomez-Ruiz, S; Lonneck, P; Silaghi-Dumitrescu, I; Silaghi-Dumitrescu, L; Hey-Hawkins, E
NEW JOURNAL OF CHEMISTRY 33 (8):1771-1779 2009
11. 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, RB; Silaghi-Dumitrescu, I; Uta, MM
INORGANIC CHEMISTRY 48 (17):8508-8514 2009
12. From closo to isocloso Structures and Beyond in Cobaltaboranes with 9 to 12 Vertices
King, RB; Silaghi-Dumitrescu, I; Sovago, I
INORGANIC CHEMISTRY 48 (21):10117-10125 2009
13. Butterfly and rhombus structures for binuclear cobalt carbonyl sulfur and phosphinidene complexes of the type Co-2(CO)(6)E-2 (E = S, PX)
Li, GL; Li, QS; Silaghi-Dumitrescu, I; King, RB; Schaefer, HF
DALTON TRANSACTIONS (47):10474-10480 2009
14. LOWER RIM SILYL SUBSTITUTED CALIX[8]ARENES
Fleuret, N; Paic, S; Nemes, G; Septelean, R; Petrar, P; Silaghi-Dumitrescu, I
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 54 (3):81-88 2009
15. Interplay among tetrahedrane, butterfly diradical, and planar rhombus structures in the chemistry of the binuclear iron carbonyl phosphinidene complexes Fe-2(CO)(6)(PX)(2)
Silaghi-Dumitrescu, I; Bitterwolf, TE; King, RB
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 130 (3):901-906 2008
16. Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes
King, RB; Silaghi-Dumitrescu, I; Uta, MM
JOURNAL OF CHEMICAL THEORY AND COMPUTATION 4 (1):209-215 2008
17. Polyhedral structures with three-, four-, and five fold symmetry in metal-centered ten-vertex germanium clusters
King, RB; Silaghi-Dumitrescu, I; Uta, MM
CHEMISTRY-A EUROPEAN JOURNAL 14 (15):4542-4550 2008
18. Bis(phosphanyl amino) benzene ligands: a zinc(II) complex and an unusual nickel(I) complex with a Dewar-benzene-type Ni₂P₂N₂ backbone
Majoum-Mbe, F; Kuhl, O; Lonneck, P; Silaghi-Dumitrescu, I; Hey-Hawkins, E
DALTON TRANSACTIONS (23):3107-3114 2008
19. Serinolic amino-s-triazines: Iterative synthesis of N-substituted amino-1,3-dioxane derivatives from l-(p-nitrophenyl)serinols and rotational stereochemistry phenomena
Fazekas, M; Pintea, M; Lameiras, P; Lesur, A; Berghian, C; Silaghi-Dumitrescu, I; Ple, N; Darabantu, M
EUROPEAN JOURNAL OF ORGANIC CHEMISTRY (14):2473-2494 2008
20. Temperature induced rotation in a [4.4]cyclophane
Bogdan, ND; Condamine, E; Toupet, L; Ramondenc, Y; Silaghi-Dumitrescu, I; Grosu, I
TETRAHEDRON LETTERS 49 (35):5204-5207 2008
21. Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-substituted derivatives of 2-aminopropane-1,3-diols
Pintea, M; Fazekas, M; Lameiras, P; Cadis, I; Berghian, C; Silaghi-Dumitrescu, I; Popa, F; Bele, C; Ple, N; Darabantu, M
TETRAHEDRON 64 (37):8851-8870 2008

22. Beyond the icosahedron: A density functional theory study of 14-atom germanium clusters
King, RB; Silaghi-Dumitrescu, I; Uta, MM
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY (25):3996-4003 2008
23. Synthesis and characterisation of some copper oxide catalysts for ozone decomposition
Dan, C; Popovici, EJ; Imre-Lucaci, F; Popovici, N; Marginean, P; Silaghi-Dumitrescu, I
JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS 10 (9):2234-2236 2008
24. 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, RB; Silaghi-Dumitrescu, I
DALTON TRANSACTIONS (44):6083-6088 2008
25. When Arsine Makes the Difference: Chelating Phosphino and Bridging Arsinoarylthiolato Gallium Complexes
Valean, AM; Gomez-Ruiz, S; Lonneck, P; Silaghi-Dumitrescu, I; Silaghi-Dumitrescu, L; Hey-Hawkins, E
INORGANIC CHEMISTRY 47 (23):11284-11293 2008
26. GERMANIUM CLUSTER POLYHEDRA
Silaghi-Dumitrescu, I; King, B
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 53 (2):83-88 2008
27. Density functional theory study of twelve-atom germanium clusters: conflict between the Wade-Mingos rules and optimum vertex degrees
King, RB; Silaghi-Dumitrescu, I; Uta, MM
DALTON TRANSACTIONS 364-372 2007
28. 1,3-digermacyclobutanes with exocyclic C=P and C=P=S double bonds
Petrar, PM; Nemes, G; Silaghi-Dumitrescu, I; Ranaivonjatovo, H; Gornitzka, H; Escudie, J
CHEMICAL COMMUNICATIONS 4149-4151 2007
29. Synthesis and characterization of calix[4]arene with different donor groups at the "NARROW" RIM
Saponar, A; Silaghi-Dumitrescu, I; Popovici, EJ; Popovici, N
REVISTA DE CHIMIE 58 (5):481-483 2007
30. 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)(PrO)-Pr-i)PS₂-S](2), and Me₂Ge{[(C₆H₅)₃SiO](p-MeOC₆H₄)PS₂-S}(2)
Fild, M; Kruger, O; Silaghi-Dumitrescu, I; Thone, C; Weinkauff, A
PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS 1822283-2310 2007
31. New digermylalkenes and digermylalkynes: [1,3]-chlorine shifts in organogermanium chemistry?
Nemes, G; Escudie, J; Silaghi-Dumitrescu, I; Ranaivonjatovo, H; Silaghi-Dumitrescu, L; Gornitzka, H
ORGANOMETALLICS 265136-5139 2007
32. cis-μ-1,4-diphenyl-1,4-diphosphorinane-κ_{P-2}: P'-bis[pentacarbonylchromium(0)] deuteriochloroform solvate
Fild, M; Krueger, ON; Silaghi-Dumitrescu, I; Thone, C; Weinkauff, A
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE 63M3011-U1347 2007
33. 1,1,4,4-Tetrabenzyl-1,4-diphosphinane-1,4-dium dibromide deuteriochloroform disolvate
Fild, M; Krueger, ON; Silaghi-Dumitrescu, I; Thone, C
ACTA CRYSTALLOGRAPHICA SECTION E-STRUCTURE REPORTS ONLINE 63O4525-U3344 2007
34. Calix[n]arene derivatives with binding properties toward Eu³⁺
Saponar, A; Silaghi-Dumitrescu, I; Popovici, EJ; Popovici, N
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (4):67-74 2007
35. Towards new double-bonded organophosphorus derivatives of C=P=C=P type
Nemes, G; Septelean, R; Petrar, PM; Silaghi-Dumitrescu, L; Silaghi-Dumitrescu, I
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (4):89-94 2007
36. Synthesis and characterization of some mixed ligand zinc(II) complexes of theophylline
Mihaly, B; Forizs, E; Silaghi-Dumitrescu, I
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (4):111-116 2007

37. Secondary interactions in heteroallenic systems with P = C-E units
Nemes, G; Silaghi-Dumitrescu, I; Petrar, PM; Septelean, R; Silaghi-Dumitrescu, L
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (1):3-9 2007
38. The formylation of bis-(N-alkyl-phenothiazinyl)-methane; A theoretical approach
Porumb, D; Silaghi-Dumitrescu, I; Gaina, L; Silaghi-Dumitrescu, L; Cristea, C; Cormos, G
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (4):39-42 2007
39. Studies on some ozone decomposition catalysts based on nickel oxide
Dan, C; Popovici, EJ; Imre, F; Indrea, E; Marginean, P; Silaghi-Dumitrescu, I
STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA 52 (1):91-95 2007
40. alpha-(3,7-Dioxa-r-1-azabicyclo[3.3.0]oct-c-5-ylmethoxy)-diazines. Part 2: Functionalisation via directed ortho-metallation and cross-coupling reactions
Berghian, C; Condamine, E; Ple, N; Turck, A; Silaghi-Dumitrescu, I; Maieranu, C; Darabantu, M
TETRAHEDRON 62 (31):7339-7354 2006
41. Molecular rotors: Design, synthesis, structural analysis, and silver complex of new [7.7] cyclophanes
Bogdan, N; Grosu, I; Benoit, G; Toupet, L; Ramondenc, Y; Condamine, E; Silaghi-Dumitrescu, I; Ple, G
ORGANIC LETTERS 8 (12):2619-2622 2006
42. First synthesis of a G-2 melamine dendrimer with serinolic peripheral groups
Darabantu, M; Pintea, M; Fazekas, M; Lameiras, P; Berghian, C; Delhom, I; Silaghi-Dumitrescu, I; Ple, N; Turck, A
LETTERS IN ORGANIC CHEMISTRY 3 (12):905-910 2006
43. 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, A; Loncke, P; Silaghi-Dumitrescu, L; Silaghi-Dumitrescu, I; Hey-Hawkins, E
DALTON TRANSACTIONS (7):967-974 2006
44. New low symmetry low energy structures of 11-atom bare germanium clusters: A density functional theory study
King, RB; Silaghi-Dumitrescu, I; Lupan, A
CHEMICAL PHYSICS 327 (2-3):344-350 2006
45. Density functional theory study of 10-atom germanium clusters: Effect of electron count on cluster geometry
King, RB; Silaghi-Dumitrescu, I; Uta, MM
INORGANIC CHEMISTRY 45 (13):4974-4981 2006
46. Structural, energetic and electronic characterization of the chiral carbon-nitride nanotubes
Rada, S; Silaghi-Dumitrescu, I
REVUE ROUMAINE DE CHIMIE 51 (2):141-145 2006
47. Phosphavinylidene(oxo)phosphorane Mes*P(O)=C=PMes*: A diphosphaallene featuring lambda(5)sigma(3)- and lambda(3)sigma(2)-phosphorus atoms
Septelean, R; Ranaivonjatovo, H; Nemes, G; Escudie, J; Silaghi-Dumitrescu, I; Gornitzka, H; Silaghi-Dumitrescu, L; Massou, S
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY 4237-4241 2006
48. Butterfly diradical intermediates in photochemical reactions of Fe-2(CO)(6)(mu-S-2)
Silaghi-Dumitrescu, I; Bitterwolf, TE; King, RB
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (16):5342-5343 2006
49. Density functional theory study of eight-atom germanium clusters: effect of electron count on cluster geometry
King, RB; Silaghi-Dumitrescu, I; Lupan, A
DALTON TRANSACTIONS (10):1858-1864 2005
50. 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 16 (4):369-377 2005
51. Density functional theory study of 11-atom germanium clusters: Effect of electron count on cluster geometry
King, RB; Silaghi-Dumitrescu, I; Lupan, A

INORGANIC CHEMISTRY 44 (10):3579-3588 2005

52. Density functional study of 8-and 11-vertex polyhedral borane structures: Comparison with bare germanium clusters

King, RB; Silaghi-Dumitrescu, I; Lupan, A
INORGANIC CHEMISTRY 44 (22):7819-7824 2005

53. A surprisingly stable 1-(chlorosilyl)-2-phosphaethyllithium compound, $\text{RCl}_2\text{SiC}(\text{Li})=\text{PMes}$
Nemes, GC; Ranaivonjatovo, H; Escudie, J; Silaghi-Dumitrescu, I; Silaghi-Dumitrescu, L; Gornitzka, H
EUROPEAN JOURNAL OF INORGANIC CHEMISTRY (6):1109-1113 2005

54. Difluorenylsilanes, -germanes, and -stannanes exhibiting an unprecedented parallel arrangement of the fluorene units

Nemes, GC; Silaghi-Dumitrescu, L; Silaghi-Dumitrescu, I; Escudie, J; Ranaivonjatovo, H; Molloy, KC; Mahon, MF; Zukerman-Schpector, J
ORGANOMETALLICS 24 (6):1134-1144 2005

55. Anodic oxidation of difluorenyls bridged through a dimethylsilyl group and of the 9-trimethylsilyl fluorene: Towards new three-dimensional polyfluorenes

Silaghi-Dumitrescu, I; Escudie, J; Cretiu-Nemes, G; Raoult, E; Rault-Berthelot, J
SYNTHETIC METALS 151 (2):114-119 2005

56. Adsorption of 6-mercaptapurine and 6-mercaptapurine riboside on silver colloid: a pH dependent surface enhanced Raman spectroscopy and density functional theory study. Part I. 6-Mercaptapurine

Szeghalmi, AV; Leopold, L; Pinzaru, S; Chis, V; Silaghi-Dumitrescu, I; Schmitt, M; Popp, J; Kiefer, W
JOURNAL OF MOLECULAR STRUCTURE 735103-113 SI 200558.

57. Adsorption of 6-mercaptapurine and 6-mercaptapurine-riboside on silver colloid: A pH-dependent surface-enhanced Raman spectroscopy and density functional theory study. II. 6-Mercaptapurine-riboside

Szeghalmi, AV; Leopold, L; Pinzaru, S; Chis, V; Silaghi-Dumitrescu, I; Schmitt, M; Popp, J; Kiefer, W
BIOPOLYMERS 78 (6):298-310 2005

2. Articole științifice publicate în ISI proceedings

3. Articole științifice indexate în BDI (din lista CNCSIS)

4. Alte articole științifice/capitole publicate în reviste/volume cu referenți (peer-reviewed)

4.1. Germanium cluster polyhedra: A density functional theory study

Silaghi-Dumitrescu, I; Kun, A; Lupan, A; King, RB
Advances in Computational Methods in Sciences and Engineering 2005, Vols 4 A & 4 B 4A-4B804-806 2005

5. Cărți științifice publicate în edituri internaționale

5.1. Theoretical Aspects of Main Group Multiple Bonded Systems, I.Silaghi-Dumitrescu, P. Petrar, G. Nemeș, R. B. King, *Computational Inorganic and Bioinorganic Chemistry*, Edward I. Solomon (Editor), Robert A. Scott (Co-Editor), R Bruce King (Co-Editor), John Wiley & Sons, pp.1-13, **2009**. ISBN: 978-0-470-69997-3. - *capitol de carte*

6. Cărți științifice publicate în edituri naționale acreditate

7. Editor de volume publicate în edituri naționale și internaționale

8. Brevete internaționale

9. Brevete naționale

10. Impact tehnologic al brevetelor: resurse financiare extrabugetare atrase în relație cu economia

11. Realizări artistice naționale și internaționale (Domeniul Arte)
(Expoziții, spectacole, concerte, publicații, filme, înregistrări)

Criteriul II – Prestigiu profesional

1. Citări ale articolelor ISI listate la Criteriul I

1. Endohedral Nickel, Palladium, and Platinum Atoms in 10-Vertex Germanium Clusters: Competition between Bicapped Square Antiprismatic and Pentagonal Prismatic Structures

Citari: 1

Title: Synthesis and Isolation of [Fe@Ge-10](3-): A Pentagonal Prismatic Zintl Ion Cage Encapsulating an Interstitial Iron Atom

Author(s): Zhou BB, Denning MS, Kays DL, et al. Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **131** Issue: **8** Pages: **2802-+** Published: **MAR 4 2009**

2. The role of "external" lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model

Citari: 3

Title: THEORETICAL CHEMISTRY Magnetic superatoms

Author(s): King B Source: **NATURE CHEMISTRY** Volume: **1** Issue: **4** Pages: **260-261** Published: **JUL 2009**

Title: The Shape of Germanium Clusters To Come

Author(s): Korber N Source: **ANGEWANDTE CHEMIE-INTERNATIONAL**

EDITION Volume: **48** Issue: **18** Pages: **3216-3217** Published: **2009**

Title: Endohedral Nickel, Palladium, and Platinum Atoms in 10-Vertex Germanium Clusters: Competition between Bicapped Square Antiprismatic and Pentagonal Prismatic Structures

Author(s): King RB, Silaghi-Dumitrescu I, Uta A M Source: **JOURNAL OF PHYSICAL CHEMISTRY**

A Volume: **113** Issue: **3** Pages: **527-533** Published: **JAN 22 2009**

3. Temperature induced rotation in a [4.4]cyclophane

Citari: 1

Title: Reinvestigation of Supramolecular Complexes with Cyclophanes of the Stetter and Koga Type: Agreement and Disagreement with Solid-State Structures

Author(s): Wald P, Schneider H J Source: **EUROPEAN JOURNAL OF ORGANIC**

CHEMISTRY Issue: **20** Pages: **3450-3453** Published: **JUL 2009**

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

Citari: 1

Title: Sterically Demanding Aminophosphines: Palladium and Gold Complexes of 1,2-

Bis(dimesitylphosphanyl amino)benzene

Author(s): Majoum Mbe F, Lonneck P, Hey-Hawkins E Source: **ZEITSCHRIFT FUR ANORGANISCHE UND**

ALLGEMEINE CHEMIE Volume: **634** Issue: **12-13** Pages: **2385-2390** Published: **2008**

5. Serinolic amino-s-triazines: Iterative synthesis of N-substituted amino-1,3-dioxane derivatives from 1-(p-nitrophenyl)serinols and rotational stereochemistry phenomena

Citari: 5

Title: Microwave-assisted synthesis of pyrazolyl bistriazines

Author(s): Moral M, Ruiz A, Moreno A, et al. Source: **TETRAHEDRON** Volume: **66** Issue: **1** Pages: **121-**

127 Published: **JAN 2 2010**

Title: SYNTHESIS OF NEW POTENTIAL DENDRITIC CORES: (4-OXOPIPERIDIN-1-YL)-s-TRIAZINES

Author(s): Popa F, Simioanca I, Pinteana M, et al. Source: **STUDIA UNIVERSITATIS BABES-BOLYAI**

CHEMIA Volume: **53** Issue: **4** Pages: **5-13** Published: **2008**

Title: NOVEL SERINOLIC MELAMINES AS POTENTIAL PERIPHERAL GROUPS IN DENDRITIC CHEMISTRY

Author(s): Darabantu M, Boulitreau L, Olosutean I, et al. Source: **STUDIA UNIVERSITATIS BABES-BOLYAI**

CHEMIA Volume: **53** Issue: **4** Pages: **21-34** Published: **2008**

Title: SYNTHESIS OF A G-2 MELAMINE BASED DENDRON HAVING 2-AMINO-2-METHYLPROPANOL UNITS AS PERIPHERAL GROUPS

Author(s): Zoltan A, Batiu C, Darabantu M Source: **STUDIA UNIVERSITATIS BABES-BOLYAI**

CHEMIA Volume: **53** Issue: **4** Pages: **51-65** Published: **2008**

Title: Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-substituted derivatives of 2-aminopropane-1,3-diols

Author(s): Pinteau M, Fazekas M, Larneiras P, et al.
Source: **TETRAHEDRON** Volume: **64** Issue: **37** Pages: **8851-8870** Published: **SEP 8 2008**

6. Polyhedral structures with three-, four-, and five fold symmetry in metal-centered ten-vertex germanium clusters
Citari: 4

Title: Polyhedral nine-atom clusters of tetrel elements and intermetalloid derivatives

Author(s): Scharfe S, Fassler TF
Source: **PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES** Volume: **368** Issue: **1915** Pages: **1265-1284** Published: **MAR 28 20**

Title: The Unique Palladium-Centered Pentagonal Antiprismatic Cationic Bismuth Cluster: A Comparison of Related Metal-Centered 10-Vertex Prictogen Cluster Structures by Density Functional Theory

Author(s): King RB, Silaghi-Dumitrescu I, Uta MM
Source: **INORGANIC CHEMISTRY** Volume: **48** Issue: **17** Pages: **8508-8514** Published: **SEP 7 2009**

Title: The Shape of Germanium Clusters To Come

Author(s): Korber N
Source: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **48** Issue: **18** Pages: **3216-3217** Published: **2009**

Title: Solid state chemistry 2008

Author(s): Moller A, Schmidt P, Wilkening M
Source: **NACHRICHTEN AUS DER CHEMIE** Volume: **57** Issue: **3** Pages: **239-251** Published: **MAR 2009**

7. Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes

Citari: 1

Title: Twelve One-Electron Ligands Coordinating One Metal Center: Structure and Bonding of [Mo(ZnCH₃)(9)(ZnCp*)(3)]

Author(s): Cadenbach T, Bollermann T, Gemel C, et al.
Source: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **47** Issue: **47** Pages: **9150-9154** Published: **2008**

8. Interplay among tetrahedrane, butterfly diradical, and planar rhombus structures in the chemistry of the binuclear iron carbonyl phosphinidene complexes Fe-2(CO)(6)(PX)(2)

Citari: 2

Title: Binuclear cyclopentadienylcobalt sulfur and phosphinidene complexes Cp₂Co₂E₂ (E = S, PX): Comparison with their Iron carbonyl analogues

Author(s): Li GL, Li QS, Silaghi-Dumitrescu I, et al.
Source: **JOURNAL OF ORGANOMETALLIC CHEMISTRY** Volume: **695** Issue: **6** Pages: **804-808** Published: **MAR 15 2010**

Title: Ionic-Type Reactivity of 1,3-Dibora-2,4-diphosphoniocyclobutane-1,3-diyls: Regio- and Stereoselective Addition of Hydracids

Author(s): Fuks G, Saffon N, Maron L, et al.
Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **131** Issue: **38** Pages: **13681-13689** Published: **SEP 30 2009**

9. First synthesis of a G-2 melamine dendrimer with serinolic peripheral groups

Citari: 8

Title: SYNTHESIS OF NEW POTENTIAL DENDRITIC CORES: (4-OXOPIPERIDIN-1-YL)-s-TRIAZINES

Author(s): Popa F, Simioanca I, Pinteau M, et al.
Source: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **53** Issue: **4** Pages: **5-13** Published: **2008**

Title: NOVEL SERINOLIC MELAMINES AS POTENTIAL PERIPHERAL GROUPS IN DENDRITIC CHEMISTRY

Author(s): Darabantu M, Boulitreau L, Olosutean I, et al.
Source: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **53** Issue: **4** Pages: **21-34** Published: **2008**

Title: SYNTHESIS OF A G-2 MELAMINE BASED DENDRON HAVING 2-AMINO-2-METHYLPROPANOL UNITS AS PERIPHERAL GROUPS

Author(s): Zoltan A, Batiu C, Darabantu M
Source: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **53** Issue: **4** Pages: **51-65** Published: **2008**

Title: An Overview of Highly Optically Pure Chloramphenicol Bases: Applications and Modifications

Author(s): Yang KH, Fang H, Gong JZ, et al.
Source: **MINI-REVIEWS IN MEDICINAL CHEMISTRY** Volume: **9** Issue: **11** Pages: **1329-1341** Published: **OCT 2009**

Title: Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-substituted

derivatives of 2-aminopropane-1,3-diols

Author(s): Pintea M, Fazekas M, Lameiras P, et

al.Source: **TETRAHEDRON** Volume: **64** Issue: **37** Pages: **8851-8870** Published: **SEP 8 2008**

Title: Serinolic amino-s-triazines: Iterative synthesis of N-substituted amino-1,3-dioxane derivatives from 1-(p-nitrophenyl)serinols and rotational stereochemistry phenomena

Author(s): Fazekas M, Pintea M, Lameiras P, et al.Source: **EUROPEAN JOURNAL OF ORGANIC CHEMISTRY** Issue: **14** Pages: **2473-2494** Published: **MAY 2008**

Title: Electrochemical behavior of a new s-triazine-based dendrimer

Author(s): Lates V, Gligor D, Darabantu M, et al.Source: **JOURNAL OF APPLIED**

ELECTROCHEMISTRY Volume: **37** Issue: **5** Pages: **631-636** Published: **MAY 2007**

10. Phosphavinylidene(oxo)phosphorane Mes*P(O)=C=PMes*: A diphosphaallene featuring lambda(5)sigma(3)- and lambda(3)sigma(2)-phosphorus atoms

Citari: 3

Title: Towards new double-bonded organophosphorus derivatives of C=P=C=P type

Author(s): Nemes G, Septelean R, Petrar PM, et al.Source: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **52** Issue: **4** Pages: **89-94** Published: **2007**

Title: Synthesis and characterization of the first arsanylbis(methylene)phosphorane (Me3Si)(2)C=P(Mes)=C(Cl)-As(F)Mes

Author(s): Petrar PM, Nemes G, Silaghi-Dumitrescu L, et al.Source: **REVUE ROUMAINE DE**

CHIMIE Volume: **52** Issue: **1-2** Pages: **45-49** Published: **JAN-FEB 2007**

Title: Group 14 and 15 heteroallenes E=C=C and E=C=E '

Author(s): Escudie J, Ranaivonjatovo HSource: **ORGANOMETALLICS** Volume: **26** Issue: **7** Pages: **1542-1559** Published: **MAR 26 2007**

11. Density functional theory study of twelve-atom germanium clusters: conflict between the Wade-Mingos rules and optimum vertex degrees

Citari: 4

Title: The Unique Palladium-Centered Pentagonal Antiprismatic Cationic Bismuth Cluster: A Comparison of Related Metal-Centered 10-Vertex Pnictogen Cluster Structures by Density Functional Theory

Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **INORGANIC**

CHEMISTRY Volume: **48** Issue: **17** Pages: **8508-8514** Published: **SEP 7 2009**

Title: The role of "external" lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model

Author(s): King RB, Silaghi-Dumitrescu ISource: **DALTON TRANSACTIONS** Issue: **44** Pages: **6083-6088** Published: **200**

Title: Beyond the icosahedron: A density functional theory study of 14-atom germanium clusters

Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **EUROPEAN JOURNAL OF INORGANIC CHEMISTRY** Issue: **25** Pages: **3996-4003** Published: **SEP 2008**

Title: Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes

Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **JOURNAL OF CHEMICAL THEORY AND COMPUTATION** Volume: **4** Issue: **1** Pages: **209-215** Published: **JAN 2**

12. Title: New low symmetry low energy structures of 11-atom bare germanium clusters: A density functional theory study

Citari: 1

Title: Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes

Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **JOURNAL OF CHEMICAL THEORY AND COMPUTATION** Volume: **4** Issue: **1** Pages: **209-215** Published: **JAN 2008**

13. alpha-(3,7-Dioxa-r-1-azabicyclo[3.3.0]oct-c-5-ylmethoxy)-diazines. Part 2: Functionalisation via directed ortho-metallation and cross-coupling reactions
Citari: 4

Title: Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-substituted derivatives of 2-aminopropane-1,3-diols
Author(s): Pintea M, Fazekas M, Lameiras P, et al.
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Title: Serinolic amino-s-triazines: Iterative synthesis of N-substituted amino-1,3-dioxane derivatives from l-(p-nitrophenyl)serinols and rotational stereochemistry phenomena
Author(s): Fazekas M, Pintea M, Lameiras P, et al.
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Title: Combined metalation-cross coupling strategies: A synthesis of schumanniohytine by a key biaryl O-carbamate remote anionic fries rearrangement
Author(s): Macklin TK, Reed MA, Snieckus V
Source: **EUROPEAN JOURNAL OF ORGANIC CHEMISTRY** Issue: **9** Pages: **1507-1509** Published: **MAR 2008**

Title: Functionalization of diazines and benzo derivatives through deprotonated intermediates
Author(s): Chevallier F, Mongin F
Source: **CHEMICAL SOCIETY REVIEWS** Volume: **37** Issue: **3** Pages: **595-609** Published: **2008**

14. : Density functional theory study of 10-atom germanium clusters: Effect of electron count on cluster geometry
Citari: 10

Title: Polyhedral nine-atom clusters of tetrel elements and intermetaloid derivatives
Author(s): Scharfe S, Fassler T
Source: **PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES** Volume: **368** Issue: **1915** Pages: **1265-1284** Published: **MAR 28 2010**

Title: The Unique Palladium-Centered Pentagonal Antiprismatic Cationic Bismuth Cluster: A Comparison of Related Metal-Centered 10-Vertex Pnictogen Cluster Structures by Density Functional Theory
Author(s): King RB, Silaghi-Dumitrescu I, Uta M
Source: **INORGANIC CHEMISTRY** Volume: **48** Issue: **17** Pages: **8508-8514** Published: **SEP 7 2009**

Title: Helical and linear [K(As-11)](2-) chains: Role of solvent on the conformation of chains formed by Zintl anions
Author(s): Reber AC, Ugrinov A, Sen A, et al.
Source: **CHEMICAL PHYSICS LETTERS** Volume: **473** Issue: **4-6** Pages: **305-311** Published: **MAY 12 2009**

Title: The Shape of Germanium Clusters To Come
Author(s): Korber N
Source: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **48** Issue: **18** Pages: **3216-3217** Published: **2009**

Title: [Co@Ge-10](3-): An Intermetaloid Cluster with Archimedean Pentagonal Prismatic Structure
Author(s): Wang JQ, Stegmaier S, Fassler T
Source: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **48** Issue: **11** Pages: **1998-2002** Published: **2009**

Title: Effect of Charge and Composition on the Structural Fluxionality and Stability of Nine Atom Tin-Bismuth Zintl Analogues
Author(s): Gupta U, Reber AC, Clayborne PA, et al.
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Title: The role of "external" lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model
Author(s): King RB, Silaghi-Dumitrescu I
Source: **DALTON TRANSACTIONS** Issue: **44** Pages: **6083-6088** Published: **2008**

Title: Beyond the icosahedron: A density functional theory study of 14-atom germanium clusters
Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **EUROPEAN JOURNAL OF INORGANIC CHEMISTRY** Issue: **25** Pages: **3996-4003** Published: **SEP 2008**

Title: Polyhedral structures with three-, four-, and five fold symmetry in metal-centered ten-vertex germanium clusters
Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **CHEMISTRY-A EUROPEAN JOURNAL** Volume: **14** Issue: **15** Pages: **4542-4550** Published: **2008**

Title: Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes
Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **JOURNAL OF CHEMICAL THEORY AND COMPUTATION** Volume: **4** Issue: **1** Pages: **209-215** Published: **JAN 2008**

15. Molecular rotors: Design, synthesis, structural analysis, and silver complex of new [7.7] cyclophanes Citari 8

Title: Design and Synthesis of Sn-Porphyrin Based Molecular Gates
Author(s): Guenet A, Graf E, Kyritsakas N, et al.Source: **INORGANIC CHEMISTRY** Volume: **49** Issue: **4** Pages:**1872-1883** Published: **FEB 15 2010**

Title: A Computational Study of Tetrafluoro-[2.2]Cyclophanes
Author(s): Caramori GF, Galembeck SESource: **JOURNAL OF PHYSICAL CHEMISTRY A** Volume: **112** Issue: **46** Pages: **11784-11800** Published: **NOV 20 2008**

Title: Temperature induced rotation in a [4.4]cyclophane
Author(s): Bogdan ND, Condamine E, Toupet L, et al.Source: **TETRAHEDRON LETTERS** Volume: **49** Issue: **35** Pages: **5204-5207** Published: **AUG 25 2008**

Title: New [4.4]cyclophanes: Molecular parallelograms, triangles, rhombuses, pentagons, and supramolecular constructions
Author(s): Bogdan N, Condamine E, Toupet L, et al.Source: **JOURNAL OF ORGANIC CHEMISTRY** Volume: **73** Issue: **15** Pages: **5831-5838** Published: **AUG 1 2008**

Title: Unsaturated strained cyclophanes based on dibenz[a,j]anthracene by an intramolecular McMurry olefination
Author(s): Chen HB, Yin J, Wang Y, et al.Source: **ORGANIC LETTERS** Volume: **10** Issue: **14** Pages: **3113-3116** Published: **JUL 17 2008**

Title: Molecular rotors as simple models to study amide NH - Aromatic interactions and their role in the folding of peptide-like structures
Author(s): Alfonso I, Burguete MI, Galindo F, et al.Source: **JOURNAL OF ORGANIC CHEMISTRY** Volume: **72** Issue:**21** Pages: **7947-7956** Published: **OCT 12 2007**

Title: New [4.4]Cyclophane diketals, monoketones, and diketones: Design, synthesis, and structural analysis
Author(s): Bogdan N, Grosu I, Condamine E, et al.Source: **EUROPEAN JOURNAL OF ORGANIC CHEMISTRY** Issue:**28** Pages: **4674-4687** Published: **OCT 2007**

Title: Synthesis and stereochemistry of some new 1,3,5-tris(1,3-dioxan-2-yl)-benzene derivatives
Author(s): Florian MC, Circu M, Toupet L, et al.Source: **CENTRAL EUROPEAN JOURNAL OF CHEMISTRY** Volume: **4** Issue: **4** Pages: **808-821** Published: **DEC 2006**

16. Butterfly diradical intermediates in photochemical reactions of Fe-2(CO)(6)(mu-S-2) Citari17:

Title: Binuclear cyclopentadienylcobalt sulfur and phosphinidene complexes Cp₂Co₂E₂ (E = S, PX): Comparison with their Iron carbonyl analogues
Author(s): Li GL, Li QS, Silaghi-Dumitrescu I, et al.Source: **JOURNAL OF ORGANOMETALLIC CHEMISTRY** Volume:**695** Issue: **6** Pages: **804-808** Published: **MAR 15 2010**

Title: Metal-Metal Bonding in Binuclear Metal Carbonyls with Three Bridging Methylaminobis(difluorophosphine) Ligands: Iron, Cobalt, and Nickel Derivatives
Author(s): Zou R, Li QS, Xie YM, et al.Source: **INORGANIC CHEMISTRY** Volume: **49** Issue: **5** Pages: **2280-2289** Published: **MAR 1 2010**

Title: Binuclear Nickel Carbonyl Thiocarbonyls: Metal-Metal Multiple Bonds versus Four-Electron Donor Thiocarbonyl Groups

Author(s): Zhang Z, Li QS, Xie Y, et al. Source: **JOURNAL OF PHYSICAL CHEMISTRY A** Volume: **114** Issue: **6** Pages: **2365-2375** Published: **FEB 18 2010**

Title: Possibilities for Titanium-Titanium Multiple Bonding in Binuclear Cyclopentadienyltitanium Carbonyls: 16-Electron Metal Configurations and Four-Electron Donor Bridging Carbonyl Groups as Alternatives

Author(s): Zhang XH, Li QS, Xie YM, et al. Source: **INORGANIC CHEMISTRY** Volume: **49** Issue: **4** Pages: **1961-1975** Published: **FEB 15 2010**

Title: Butterfly and rhombus structures for binuclear cobalt carbonyl sulfur and phosphinidene complexes of the type Co-2(CO)(6)E-2 (E = S, PX)

Author(s): Li GL, Li QS, Silaghi-Dumitrescu I, et al. Source: **DALTON TRANSACTIONS** Issue: **47** Pages: **10474-10480** Published: **2009**

Title: Prospects for Making Organometallic Compounds with BF Ligands: Fluoroborylene Iron Carbonyls

Author(s): Xu LC, Li QS, Xie YM, et al. Source: **INORGANIC CHEMISTRY** Volume: **49** Issue: **3** Pages: **1046-1055** Published: **FEB 1 2010**

Title: Introducing a dark reaction to photochemistry: photocatalytic hydrogen from [FeFe] hydrogenase active site model complexes

Author(s): Lomoth R, Ott S Source: **DALTON TRANSACTIONS** Issue: **45** Pages: **9952-9959** Published: **2009**

Title: Activation of the S-H Group in Fe(μ (2)-SH)Fe Clusters: S-H Bond Strengths and Free Radical Reactivity of the Fe(μ (2)-SH)Fe Cluster

Author(s): Franz JA, Lee SJ, Bowden TA, et al. Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **131** Issue: **42** Pages: **15212-15224** Published: **OCT 28 2009**

Title: Ionic-Type Reactivity of 1,3-Dibora-2,4-diphosphoniocyclobutane-1,3-diyls: Regio- and Stereoselective Addition of Hydracids

Author(s): Fuks G, Saffon N, Maron L, et al. Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **131** Issue: **38** Pages: **13681-13689** Published: **SEP 30 2009**

Title: Binuclear Cobalt Thiocarbonyl Carbonyl Derivatives: Comparison with Homoleptic Binuclear Cobalt Carbonyls

Author(s): Zhang Z, Li QS, Xie YM, et al. Source: **INORGANIC CHEMISTRY** Volume: **48** Issue: **13** Pages: **5973-5982** Published: **JUL 6 2009**

Title: Iron Carbonyl Thiocarbonyls: Effect of Substituting a Thiocarbonyl Group for a Carbonyl Group in Mononuclear and Binuclear Iron Carbonyl Derivatives

Author(s): Zhang Z, Li OS, Xie YM, et al. Source: **INORGANIC CHEMISTRY** Volume: **48** Issue: **5** Pages: **1974-1988** Published: **MAR 2 2009**

Title: Unsaturation in binuclear benzene manganese carbonyls: Comparison with isoelectronic cyclopentadienyliron and cyclobutadienecobalt derivatives

Author(s): Wang HY, Xie YM, King RB, et al. Source: **ORGANOMETALLICS** Volume: **27** Issue: **18** Pages: **4572-4579** Published: **SEP 22 2008**

Title: Formal chromium-chromium triple bonds and bent rings in the binuclear cycloheptatrienylchromium carbonyls (C₇H₇)₂Cr-2(CO)_n (n = 6, 5, 4, 3, 2, 1, 0): A density functional theory study

Author(s): Wang HY, Xie YM, King RB, et al. Source: **JOURNAL OF ORGANOMETALLIC CHEMISTRY** Volume: **693** Issue: **20** Pages: **3201-3212** Published: **OCT 1 2008**

Title: Multiple-timescale photoreactivity of a model compound related to the active site of [FeFe]-hydrogenase

Author(s): Ridley AR, Stewart AI, Adamczyk K, et al. Source: **INORGANIC CHEMISTRY** Volume: **47** Issue: **17** Pages: **7453-7455** Published: **SEP 1 2008**

Title: Refining the active site structure of iron-iron hydrogenase using computational infrared spectroscopy
Author(s): Tye JW, Darensbourg MY, Hall MBSource: **INORGANIC CHEMISTRY** Volume: **47** Issue: **7** Pages:**2380-2388** Published: **APR 7 2008**

Title: Interplay among tetrahedrane, butterfly diradical, and planar rhombus structures in the chemistry of the binuclear iron carbonyl phosphinidene complexes Fe-2(CO)(6)(PX)(2)
Author(s): Silaghi-Dumitrescu I, Bitterwolf TE, King RBSource: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **130** Issue: **3** Pages: **901-906** Published: **JAN 23 2008**

Title: Spectroscopic detection and theoretical confirmation of the role of Cr-2(CO)(5)(C5R5)(2) and center dot Cr(CO)(2)(ketene)(C5R5) as intermediates in carbonylation of N=N=CHSiMe3 to O=C=CHSiMe3 by center dot Cr(CO)(3)(C5R5) (R = h, CH3)
Author(s): Fortman GC, Kegl T, Li QS, et al.Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume:**129** Issue: **46** Pages: **14388-14400** Published: **NOV 21 2007**

17. 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)

Citari: 5

Title: Synthesis and structural characterization of a mixed aggregate containing a lithium thiolate and a lithium amide
Author(s): Goto K, Takahashi Y, Kawashima TSource: **JOURNAL OF SULFUR CHEMISTRY** Volume: **30** Issue: **3-4** Special Issue: **Sp. Iss. SI** Pages: **365-369** Published: **2009**

Title: Bis(phosphanyl amino) benzene ligands: a zinc(II) complex and an unusual nickel(I) complex with a Dewar-benzene-type Ni2P2N2 backbone
Author(s): Majoumo-Mbe F, Kuhl O, Lonnecke P, et al.Source: **DALTON TRANSACTIONS** Issue: **23** Pages: **3107-3114** Published: **200**

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Author(s): Strohmann C, Gessner VHSsource: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **46** Issue:**24** Pages: **4566-4569** Published: **2007**

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Author(s): Bojer D, Kamps I, Tian X, et al.Source: **ANGEWANDTE CHEMIE-INTERNATIONAL EDITION** Volume: **46** Issue: **22** Pages: **4176-4179** Published: **2007**

Title: New reactivity and structural insights of alkali-metal-mediated aluminations in directed ortho-alumination of a tertiary aromatic amide
Author(s): Garcia-Alvarez J, Graham DV, Kennedy AR, et al.Source: **CHEMICAL COMMUNICATIONS** Issue: **30** Pages: **3208-3210** Published: **2006**

18. Title: Density functional theory study of eight-atom germanium clusters: effect of electron count on cluster geometry
Citari: 10

Title: The Unique Palladium-Centered Pentagonal Antiprismatic Cationic Bismuth Cluster: A Comparison of Related Metal-Centered 10-Vertex Pnictogen Cluster Structures by Density Functional Theory
Author(s): King RB, Silaghi-Dumitrescu I, Uta MMSource: **INORGANIC CHEMISTRY** Volume: **48** Issue: **17** Pages:**8508-8514** Published: **SEP 7 2009**

Title: GERMANIUM CLUSTER POLYHEDRA
Author(s): Silaghi-Dumitrescu I, King BSource: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **53** Issue: **2** Pages: **83-88** Published: **2008**

Title: Effect of Charge and Composition on the Structural Fluxionality and Stability of Nine Atom Tin-Bismuth Zintl Analogues
Author(s): Gupta U, Reber AC, Clayborne PA, et al.Source: **INORGANIC CHEMISTRY** Volume: **47** Issue: **23** Pages: **10953-10958** Published: **DEC 1 2008**

Title: The role of "external" lone pairs in the chemical bonding of bare post-transition element clusters: the Wade-Mingos rules versus the jellium model

Author(s): King RB, Silaghi-Dumitrescu I Source: **DALTON TRANSACTIONS** Issue: **44** Pages: **6083-6088** Published: **2008**

Title: Singly bonded catenated germanes: Eighty years of progress

Author(s): Amadoruge ML, Weinert CS Source: **CHEMICAL REVIEWS** Volume: **108** Issue: **10** Pages: **4253-4294** Published: **OCT 2008**

Title: Beyond the icosahedron: A density functional theory study of 14-atom germanium clusters

Author(s): King RB, Silaghi-Dumitrescu I, Uta MM Source: **EUROPEAN JOURNAL OF INORGANIC CHEMISTRY** Issue: **25** Pages: **3996-4003** Published: **SEP 2008**

Title: Beyond the Wade-Mingos rules in bare 10- and 12-vertex germanium clusters: Transition states for symmetry breaking processes

Author(s): King RB, Silaghi-Dumitrescu I, Uta MM Source: **JOURNAL OF CHEMICAL THEORY AND COMPUTATION** Volume: **4** Issue: **1** Pages: **209-215** Published: **JAN 2008**

Title: Density functional theory study of twelve-atom germanium clusters: conflict between the Wade-Mingos rules and optimum vertex degrees

Author(s): King RB, Silaghi-Dumitrescu I, Uta MM Source: **DALTON TRANSACTIONS** Issue: **3** Pages: **364-372** Published: **2007**

Title: Density functional theory study of 10-atom germanium clusters: Effect of electron count on cluster geometry

Author(s): King RB, Silaghi-Dumitrescu I, Uta MM Source: **INORGANIC CHEMISTRY** Volume: **45** Issue: **13** Pages: **4974-4981** Published: **JUN 26 2006**

Title: Rules for counting electrons and three-dimensional aromaticity

Author(s): Shainyan BA Source: **RUSSIAN JOURNAL OF ORGANIC CHEMISTRY** Volume: **42** Issue: **2** Pages: **304-306** Published: **FEB 2006**

19. Density functional study of 8- and 11-vertex polyhedral borane structures: Comparison with bare germanium clusters

Citari: 3

Title: GERMANIUM CLUSTER POLYHEDRA

Author(s): Silaghi-Dumitrescu I, King B Source: **STUDIA UNIVERSITATIS BABES-BOLYAI CHEMIA** Volume: **53** Issue: **2** Pages: **83-88** Published: **2008**

Title: Effects of halogen substitution on the properties of eight- and nine-vertex closo-boranes

Author(s): Corminboeuf C, Wodrich MD, King RB, et al. Source: **DALTON TRANSACTIONS** Issue: **13** Pages: **1745-1751** Published: **APR 7 2008**

Title: First-principles study on the stability of intermediate compounds of LiBH₄

Author(s): Ohba N, Miwa K, Aoki M, et al. Source: **PHYSICAL REVIEW B** Volume: **74** Issue: **7** Article Number: **075110** Published:

20. Adsorption of 6-mercaptopurine and 6-mercaptopurine-riboside on silver colloid: A pH-dependent surface-enhanced Raman spectroscopy and density functional theory study. II. 6-Mercaptopurine-riboside

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Title: SERS Not To Be Taken for Granted in the Presence of Oxygen

Author(s): Erol M, Han Y, Stanley SK, et al. Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **131** Issue: **22** Pages: **7480+** Published: **JUN 10 2009**

Title: Time fluctuations and imaging in the SERS spectra of fungal hypha grown on nanostructured substrates

Author(s): Szeghalmi A, Kaminskyj S, Rosch P, et al. Source: **JOURNAL OF PHYSICAL CHEMISTRY B** Volume: **111** Issue: **44** Pages: **12916-12924** Published: **NOV 8 2007**

Title: Electromagnetic mechanism of SERS
Author(s): Schatz GC, Young MA, Van Duyne RP Source: **SURFACE-ENHANCED RAMAN SCATTERING: PHYSICS AND APPLICATIONS** Book Series: **TOPICS IN APPLIED PHYSICS** Volume: **103** Pages: **19-45** Published: **2006**

Title: On the experimental estimation of surface enhanced raman scattering (SERS) cross sections by vibrational pumping
Author(s): Maher RC, Cohen LF, Le Ru EC, et al. Source: **JOURNAL OF PHYSICAL CHEMISTRY B** Volume: **110** Issue: **39** Pages: **19469-19478** Published: **OCT 5 2006**

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Author(s): King RB, Silaghi-Dumitrescu I Source: **DALTON TRANSACTIONS** Issue: **44** Pages: **6083-6088** Published: **2008**

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Author(s): King RB, Silaghi-Dumitrescu I, Uta MM Source: **EUROPEAN JOURNAL OF INORGANIC CHEMISTRY** Issue: **25** Pages: **3996-4003** Published: **SEP 2008**

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Author(s): Darabantu, M; Maiereanu, C; Silaghi-Dumitrescu, I, et al.
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Author(s): Pintea M, Fazekas M, Larnearas P, et al. Source: **TETRAHEDRON** Volume: **64** Issue: **37** Pages: **8851-8870** Published: **SEP 8 2008**
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Author(s): King, RB; Silaghi-Dumitrescu, I

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 5. Author(s): Pantazis DA, McGrady JES Source: **JOURNAL OF THE AMERICAN CHEMICAL SOCIETY** Volume: **128** Issue: **12** Pages: **4128-4135** Published: **MAR 29 2006**
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 Source: **TETRAHEDRON** Volume: **56** Issue: **23** Pages: **3785-3798** Published: **JUN 2 2000**
- Title: alpha-(3,7-Dioxa-r-1-azabicyclo[3.3.0]oct-c-5-ylmethoxy)-diazines. Part 2: Functionalisation via directed ortho-metallation and cross-coupling reactions
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- Title: Ring-ring tautomerism of some spirooxazolidines derived from l-phenylserinols
 2. Author(s): Maieranu C, Darabantu M, Ple G, et al. Source: **REVUE ROUMAINE DE CHIMIE** Volume: **50** Issue: **1** Pages: **29-40** Published: **JAN 2005**
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18. Title: Synthesis and stereochemistry of some 1,3-oxazolidine systems based on TRIS (alpha,alpha,alpha-trimethylolaminomethane) and related aminopolyols skeleton. part 2: 1-aza-3,7-dioxabicyclo[3.3.0]octanes
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- Title: SERINOLIC APPROACH IN THE SYNTHESIS OF THE 3-OXA-7-THIA-1-
1. AZABICYCLO[3.3.0]OCTANE SKELETON FUNCTIONALISED AT THE C-5 POSITION
Author(s): But A, Batiu C, Ramondenc Y, et al. Source: **REVUE ROUMAINE DE CHIMIE** Volume: **54** Issue: **2** Pages: **127-132** Published: **FEB 2009**
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- Title: Serinolic amino-s-triazines: iterative synthesis and rotational stereochemistry phenomena as N-
3. substituted derivatives of 2-aminopropane-1,3-diols
Author(s): Pintea M, Fazekas M, Lameiras P, et al. Source: **TETRAHEDRON** Volume: **64** Issue: **37** Pages: **8851-8870** Published: **SEP 8 2008**
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- Title: alpha-(3,7-Dioxa-r-1-azabicyclo[3.3.0]oct-c-5-ylmethoxy)-diazines. Part 1: Synthesis and
4. stereochemistry. Extension to s-triazine series
Author(s): Berghian C, Lameiras P, Toupet L, et al. Source: **TETRAHEDRON** Volume: **62** Issue: **31** Pages: **7319-7338** Published: **JUL 31 2006**
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5. Author(s): Maieranu C, Darabantu M, Ple G, et al. Source: **REVUE ROUMAINE DE CHIMIE** Volume: **50** Issue: **1** Pages: **29-40** Published: **JAN 2005**
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- Title: First examples of the conformation chirality of heterobicyclo[3.3.0]octanes: 3,7-dioxa-r-1-
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Author(s): Berghian C, Darabantu M, Lameiras P, et al. Source: **HETEROCYCLIC COMMUNICATIONS** Volume: **11** Issue: **6** Pages: **517-522** Published: **2005**
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7. series
Author(s): Maieranu C, Darabantu M, Condamine E, et al. Source: **HETEROCYCLIC COMMUNICATIONS** Volume: **11** Issue: **3-4** Pages: **305-310** Published: **2005**
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Author(s): Maieranu C, Darabantu M, Ple G, et al. Source: **REVUE ROUMAINE DE CHIMIE** Volume: **50** Issue: **2** Pages: **103-112** Published: **FEB 2005**
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19. Title: An AM1 investigation of the structures of C60 : tBu-calix[8]arene 1 : 1 adducts
Author(s): Lara-Ochoa, F; Cogordan, JA; Cruz, R, et al.
Source: **FULLERENE SCIENCE AND TECHNOLOGY** Volume: **7** Issue: **3** Pages: **411-419** Published: **1999**
- Title: Analysis of interaction modes in calix[4]arene - levofloxacin complexes by quantum methods
1. Author(s): Lambert A, Regnouf-de-Vains JB, Rinaldi D, et al. Source: **JOURNAL OF PHYSICAL ORGANIC CHEMISTRY** Volume: **19** Issue: **3** Pages: **157-166** Published: **MAR 2006**
Times Cited: **3**
20. Title: Is the trigonal prismatic distortion the answer for the geometry of In-III four members dithiochelatate compounds? The crystal and molecular structure of In(S2AsR2)(3) (R = Me, Ph)
Author(s): Silaghi-Dumitrescu, L; Silaghi-Dumitrescu, I; Haiduc, I, et al.

- Title: Preparation and Properties of Sodium Dimethyldithioarsinate Dihydrate, $\text{Me}_2\text{AsS}_2\text{Na}$ center dot $2\text{H}_2\text{O}$, and Palladium(II) Dimethyldithioarsinate, $(\text{Me}_2\text{AsS}_2)_2\text{Pd}$
1. Author(s): Ioannou PV, Vachliotis DG, Nastopoulos V, et al. Source: **ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE** Volume: **635** Issue: **13-14** Pages: **2203-2209** Published: **2009**
Times Cited: **0**
- Title: The Lewis-base behavior of Bunsen's cacodyl disulfide, $\text{Me}_2\text{As}(\text{S})\text{-S-AsMe}_2$, toward molecular halides of group 13
2. Author(s): Ioannou PV, Tsivgoulis GM, Vachliotis DG Source: **MAIN GROUP CHEMISTRY** Volume: **8** Issue: **3** Pages: **151-161** Published: **2009**
Times Cited: **1**
- Title: Main Group Dithiocarbamate Complexes
3. Author(s): Heard PJ Source: **PROGRESS IN INORGANIC CHEMISTRY, VOL 53** Book Series: **PROGRESS IN INORGANIC CHEMISTRY** Volume: **53** Pages: **1-69** Published: **2005**
Times Cited: **26**
- Title: Gallium(III) and indium(III)dithiolate complexes: Versatile precursors for metal sulfides
4. Author(s): Ghoshal S, Jain VK Source: **JOURNAL OF CHEMICAL SCIENCES** Volume: **119** Issue: **6** Pages: **583-591** Published: **NOV 2007**
Times Cited: **2**
21. Title: 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
Author(s): Silaghi-Dumitrescu, L; Haiduc, I; Cea-Olivares, R, et al.
Source: **JOURNAL OF ORGANOMETALLIC CHEMISTRY** Volume: **545** Pages: **1-8** Published: **1997**
- Title: Silatropic migration in (1-trimethylsilylindenyl) (indenyl) dimethylsilane, bis(1-trimethylsilylindenyl)dimethylsilane and related compounds
1. Author(s): Nemes G, Silaghi-Dumitrescu L, Silaghi-Dumitrescu L, et al. Source: **REVUE ROUMAINE DE CHIMIE** Volume: **52** Issue: **8-9** Pages: **809+** Published: **AUG-SEP 2007**
Times Cited: **0**
- Title: Anodic oxidation of difluorenyls bridged through a dimethylsilyl group and of the 9-trimethylsilyl fluorene: Towards new three-dimensional polyfluorenes
2. Author(s): Silaghi-Dumitrescu I, Escudie J, Cretiu-Nemes G, et al. Source: **SYNTHETIC METALS** Volume: **151** Issue: **2** Pages: **114-119** Published: **JUN 14 2005**
Times Cited: **1**
- Title: Difluorenylsilanes, -germanes, and -stannanes exhibiting an unprecedented parallel arrangement of the fluorene units
3. Author(s): Nemes GC, Silaghi-Dumitrescu L, Silaghi-Dumitrescu I, et al. Source: **ORGANOMETALLICS** Volume: **24** Issue: **6** Pages: **1134-1144** Published: **MAR 14 2005**
Times Cited: **5**
22. Title: The first oxygen-bridged diorganoarsenic(V) compound: the crystal structure of $\text{AsMe}_2(\text{S})\text{OAs}(\text{S})\text{Me}_2$
Author(s): Silaghi-Dumitrescu, L; Pascu, S; Silaghi-Dumitrescu, I, et al.
Source: **JOURNAL OF ORGANOMETALLIC CHEMISTRY** Volume: **549** Issue: **1-2** Pages: **187-192** Published: **DEC 18 1997**
- Title: The reactions of triethylamine-activated octasulfur with thioarsinites, $\text{L}_2\text{As-SPh}$ (L = Me, Ph), Bunsen's cacodyl disulfide, $\text{Me}_2\text{As}(\text{S})\text{-S-AsMe}_2$, and triphenylarsine
1. Author(s): Sideris TD, Tsivgoulis GM, Vachliotis DG, et al. Source: **MAIN GROUP CHEMISTRY** Volume: **8** Issue: **3** Pages: **163-176** Published: **2009**
Times Cited: **0**

- Title: Synthesis, Crystal Structures and Spectroscopic Studies of Dimorphic [Bu₂Sn(O₂AsMe₂)(₂)] and the
 2. Novel Dimethylthioarsinate [(Me₂SnOSAsMe₂)(₂O)](₂)
 Author(s): Shihada AF, Al-Aqarbeh M, Weller F, et al. Source: **ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE** Volume: **635** Issue: **9-10** Pages: **1384-1390** Published: **2009**
 Times Cited: **0**
- Title: The Other Face of Bunsen's Cacodyl Disulfide, Me₂As(S)-S-AsMe₂: The Lewis-Base Behaviour
 3. Towards Heavy Metal Cations
 Author(s): Ioannou PV, Vachliotis DG, Sideris TD Source: **ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE** Volume: **635** Issue: **2** Pages: **329-336** Published: **2009**
 Times Cited: **1**
- Title: The electrophilic character of Bunsen's cacodyl disulfide, Me₂As(S)-S-AsMe₂
 4. Author(s): Ioannou PV, Vachliotis DG, Sideris TD Source: **ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE** Volume: **633** Issue: **11-12** Pages: **2077-2084** Published: **2007**
 Times Cited: **3**
- Title: Dimethylthioarsinic anhydride: A standard for arsenic speciation
 5. Author(s): Fricke M, Zeller M, Cullen W, et al. Source: **ANALYTICA CHIMICA ACTA** Volume: **583** Issue: **1** Pages: **78-83** Published: **JAN 30 2007**
 Times Cited: **8**
- Title: Chromatographic separation and identification of products from the reaction of dimethylarsinic acid
 6. with hydrogen sulfide
 Author(s): Fricke MW, Zeller M, Sun H, et al. Source: **CHEMICAL RESEARCH IN TOXICOLOGY** Volume: **18** Issue: **12** Pages: **1821-1829** Published: **DEC 2005**
 Times Cited: **23**

4. Distincții, premii și alte recunoașteri naționale și internaționale

Diploma de Merit pentru contributi la dezvoltarea institutionala a Universitatii Babes-Bolyai, 2005
 Diploma Consiliului Academic al Universitatii Babes-Bolyai, 2006, 2007.
 Membru corespondent al Academiei Romane, 2007

5. Studenți naționali atrași (activități de coordonare științifică și didactică)

- **Îndrumare lucrari de licență (număr lucrări susținute) : 20**
- Îndrumare lucrări de disertație (număr lucrări susținute) : 10
- Doctoranzi (lista nominală a doctoranzilor înmatriculați resp. lista nominală a tezelor susținute) :
- Post-doctoranzi (lista nominală) : 1

Lista nominala a doctoranzilor înmatriculați cu frecventa :

1. Kolcsor Tibor
2. Irsai Isabella
3. Sarosi Menyhardt
4. Zoltany Timea
5. Mihaly Bela
6. Sovago Ioana
7. Kekedy-Nagy Laszlo
8. Seff Amalia

Lista nominală a tezelor susținute

1. Septelean Raluca
2. Saponar Alina
3. Petrar Petronela
4. Uta Matei

5. Lupan Alexandru
6. Totos Robert
7. Furtos Gabriel

6. Studenți internaționali atrasi (activități de coordonare științifică și didactică)

- **Îndrumare lucrări de licență (număr lucrări susținute) :**
- Îndrumare lucrări de disertație (număr lucrări susținute)
- Doctoranzi (lista nominală a doctoranzilor înmatriculați resp. lista nominală a tezelor susținute)
- Post-doctoranzi (lista nominală)

Post-doctoranzi

1. Joaquin Barroso-Flores

7. Membru in comitetul de redacție la reviste ISI

1. Studia Universitatis Babes-Bolyai, Seria Chemia
2. Revista de Chimie, Bucuresti

8. Membru in comitetul de redacție la reviste BDI

9. Participări la programe/granturi de cercetare finanțate din sursă internațională (se menționează și valoarea)

- 9.1. Proiect de Cooperare bilaterala Brancusi, Heteroalcenes, –dienes et allenes precurseurs de polymeres organometaliques: acces a de nouveaux materiaux, 2004-2006, valoare 6000 E.
- 9.2. International Master and Postgraduate Programme in Materials Science and Catalysis, la University SS Cyril and Methodius, Skopje, Macedonia, 2009.

10. Participări la programe/granturi finanțate din sursă națională (se menționează și valoarea)

- 10.1. CEEX-SUPRACOM, *Chimie organometalica supramoleculara : De la design prin sinteză și structură la aplicații*, 2006-2008, 1000000 RON.
- 10.2. CEEX-RIOSIN, *Reactivi si intermediary organometalici in sinteze stereocontrolate de compusi cu relevanta biologica*, 2006-2008, valoare 1200000 RON.
- 10.3. Programul Cercetare de Excelenta OPTOLUM 2005-2007 (dir. L. Silaghi-Dumitrescu), valoare 300000 lei.
- 10.4. PN II, Capacitati I-ELANCOM, Extinderea laboratoarelor de chimie organometalica aplicata, 129/2007, 2007-2009 (dir. L. Silaghi-Dumitrescu), valoare 1859500 lei

11. Coordonări de programe/granturi finanțate din sursă internațională (se menționează și valoarea)

- 9.1. Proiect de Cooperare bilaterala Econet, 2007-2009, valoare 13000 E.

12. Coordonări de programe/granturi finanțate din sursă națională (se menționează și valoarea)

- 12.1. CEEX-Modul III, *Modelare moleculara in chimie si biochimie-MOLMOD*, 2006-2008, 200000 RON.

12.2. Proiect de cooperare bilaterală Capacități Modul III, *Studiul conformațiilor controlate cinetic ale moleculelor gazdă sensibile și selective cu aplicații în farmacie și chimie alimentară*, 2008-2009, 160443 RON.

12.3. CEEX-CALIXCOM, *Materiale compozite pe bază de calixarene cu proprietăți magnetice și/sau de complexare selectivă a unor ioni de metale de interes tehnologic*, 2005-2008, 1500000 RON.

12.4. PNII-CALIXMAT, *Materiale pe baza de calixarene cu proprietati de recunoastere a unor specii ionice si/sau moleculare de interes biologic si ecologic*, 2007-2010, 2000000 RON.

12.5. Centru de Modelare Moleculara si Chimie Cuantica computationala, PNII, Capacitati I, contract 130,2007, CCMMCCC, (Coordonator, Ioan Silaghi-Dumitrescu), valoare 1305000 RON

13. Profesor invitat la universitati de prestigiu, cu titlu oficial

Profesor invitat la Universitatea din Leipzig si Koln, Germania

14. Membru în comisii profesionale relevante, cu titlu oficial

15. Conferințe invitate internaționale

16. Membru în comitete de organizare sau științifice ale unor conferințe internaționale

1. **MOLMOD**, Molecular modeling in chemistry and biochemistry, Cluj-Napoca, 2-4 aprilie, 2009.

2. **MOLMOD**, Molecular modeling in chemistry and biochemistry, Arcalia, 5-8 iulie, 2007.

3. **SUPCHEM**, Supramolecular Chemistry from design to application, Cluj-Napoca 12-15 aprilie, 2007.

III. Realizare remarcabilă

Profesorul Silaghi-Dumitrescu Ioan a infiintat scoala de Chimie Computationala si Modelare Moleculara la Cluj-Napoca. A infiintat si dezvoltat Laboratorul de Structura si Dinamica Moleculara, Laboratorul de Modelare Moleculara si intre anii 2007-2009, cea mai moderna platforma de calcul din tara, Centrul de Modelare Moleculara si Chimie Cuantica Computationala.

Data:

17.03.2010

Semnătura:

Certific validitatea datelor prezentate

Sef de catedră,