PERSONAL INFORMATION

Alexandru Lupan



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Sex M | Date of birth 1978 | Nationality Romanian

2021 - present **Assoc. Prof. Dr. Habil. at the Faculty of Chemistry and Chemical Engineering of the Babeș-Bolyai University in Cluj-Napoca, Romania**

WORK EXPERIENCE

2017 - 2021 Lecturer

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Courses and seminars of Structural Chemistry and Molecular medicine and imagistic techniques and research activity in molecular modelling and quantum chemistry

Business or sector public university

2020 - 2022 Project director PN-III-P2-PED-2293

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Semi-artificial oxygen carriers”

Business or sector public university

2017 - 2019 Project director PN-III-P4-PCE-0089

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Molecular metal clusters: bridging the gap between small molecules and nanocrystals”

Business or sector public university

2015 - 2017 Project director PN-II-RU-TE-1197

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Polyhedral metallaboranes: metal clusters stabilized in borane matrices”

Business or sector public university

2014 - 2015 Project director GTC-334017

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Eight vertex tetrametallaboranes: intermediates between polyhedral boranes and metal clusters”

Business or sector public university

2013 - 2016 Research assistant

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Redox activation of small molecules at biologic metal centers” (PI prof. dr. Radu Silaghi-Dumitrescu)

Business or sector public university

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2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project "Biomolecule nanomanipulation by atomic force microscopy" (PI acad. prof. dr. Octavian Popescu)

Business or sector public university

2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project "Biomedical applications of metallic compounds - Metallomics" (PI acad. prof. dr. Ionel Haiduc)

Business or sector public university

2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project "Biofunctionalised nanoparticles for developing new imagistic, diagnose, and molecular therapy in biological environments" (PI prof. dr. Simion Aștilean)

Business or sector public university

2006 - 2009 **Postdoctoral researcher**

Chemistry and Biocatalysis unit, Institut Pasteur, Paris, France

- Research activity within the project IdF 06-222_09-1739/2006 "Medicen – chemical library of new chemical entities" (PI CR1 dr. Helene Munier-Lehmann)

Business or sector research institute

2006 - 2017 **Chemist**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Laboratory works in general and inorganic chemistry, molecular modeling and research activity

Business or sector public university

EDUCATION AND TRAINING

2002 - 2006 **Ph. D. in Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Electronic structure calculations of main group cluster compounds

2001 - 2002 **Master in Organometallic and Applied Coordination Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Inorganic chemistry with dissertation in molecular modeling

1997 - 2001 **B. Sc. in Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Chemistry specialisation with dissertation in coordination chemistry

1993 - 1997 **Baccalaureate**

Gheorghe Șincai High School, Cluj-Napoca, Romania

- Chemistry-Biology specialisation

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PERSONAL SKILLS

Mother tongue(s): Romanian

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C2	C2	C2	C2	C2
French	C2	C2	C2	C2	C2

Levels: A1/2: Basic user - B1/2: Independent user - C1/2 Proficient user
Common European Framework of Reference for Languages

Communication skills

- good communication skills adapted for teaching and mentoring student research activities
- good communication as member of various research teams
- adaptation to multicultural environments and collaboration with other universities

Organisational / managerial skills

- managing research activities as team leader of various research projects

Job-related skills

- good command of quality control processes and acquisitions

Computer skills

- electronic structure calculations, i.e. molecular mechanics, semiempirical, ab initio, post-Hartree Fock, DFT, NBO analysis, TD-DFT, using specialised software such as Gaussian, Gamess, Mopac, Spartan, NWChem.

Other skills

- Experimental and virtual screening techniques, enzymatic analysis and kinetics

ADDITIONAL INFORMATION

ResearcherID: http://www.researcherid.com/rid/A-3142-2012
Presentations: https://www.researchgate.net/profile/Alexandru_Lupan2
Google Scholar: https://scholar.google.com/citations?user=tU6Xp6AAAAAJ&hl=en

Publications - articles

1. "High-spin face-capped deltahedra in divanadadicarbaboranes are very different from the singlet structures of chromium analogues" H. Casian, A. Lupan*, R.B. King, Dalton Trans., 2025, 54, 12463-12470. doi: 10.1039/d5dt01520k
2. "Influence of the second coordination sphere on the autooxidation reaction in oxygen-binding proteins" A.M. Cosprundan, N. Adrian, C. Zagrean-Tuza, M. Lehene, B. Brem, E. Gal, A. Lupan, R. Silaghi-Dumitrescu, Dalton Trans., 2025, 54, 12463-12470. doi:
3. "Binuclear methylphosphinidine complexes of cyclopentadienylruthenium carbonyls: effects of the higher ligand field strength of ruthenium derivatives relative to iron derivatives" O. Rudenco, A. Lupan*, R. Silaghi-Dumitrescu, R.B. King, Dalton Trans., 2024, 53, 17654-17663. doi:10.1039/d4dt02279c
4. "An iron-free nitrogenase? Computational estimation of the ability to bind/activate N2 in manganese and cobalt complexes" R. Doukeh, D. Craciun, M. Lehene, A.M. Branzanic, A. Lupan, R. Silaghi-Dumitrescu, J. Coord. Chem., 2024, 77, 1597-1606. doi: 10.1080/00958972.2024.2372812
5. "Weak interactions between hydracids/binary acids: some considerations from a DFT analysis" L. Radu, A. Lupan, M. Lehene, , R. Silaghi-Dumitrescu, Studia Chemia, 2024, 69, 121-134. doi: 10.24193/subbchem.2024.2.09
6. "Decarbonylation products of binuclear methylphosphinidene complexes of cyclopentadienyliron carbonyls: triplet and quintet structures are favored energetically over singlet structures with iron-iron multiple bonding" O. Rudenco, A. Lupan*, R. Silaghi-Dumitrescu, R.B. King, •ACS Omega, 2024, 9, 12125-12134. doi:10.1021/acsomega.3c10460
7. "A theoretical study of the effect of phosphorus and nitrogen heteroatoms on pentahapto coordination of diazaphospholyl ligands in binuclear ruthenium and iron carbonyl derivatives" T.M. Danescu, R. A. Lupan*, Silaghi-Dumitrescu, , R.B. King, •J. Organomet. Chem., 2024, 1004, 122949; doi: 10.1016/j.jorganchem.2023.122949
8. "Dual spherical-spherical aromaticity in [M(η2-P4)2]+ (M = Cu, Ag, Au) and [P(P4)2]+. Evaluation of bonding nature and spherical aromatic character of the P4 aggregates from DFT calculations" C.O. Ulloa, A.A. Attia, A. Lupan, R.B. King, A. Munoz-Castro, •Inorg. Chem. Commun., 2024, 159, 111680; doi: 10.1016/j.inoche.2023.111680
9. "A study of the molecular interactions of hemoglobin with diverse classes of therapeutic agents" C. Zagrean-Tuza, I. Igescu, A. Lupan, R. Silaghi-Dumitrescu, •Inorg. Chim. Acta, 2024, 567, 122053 doi: 10.1016/j.ica.2024.122053

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10. "A poly(methyl methacrylate)-ibuprofen composite film as anticorrosive coating of Ti-6Al-4 V surface" J.H. Viteri, N. Cotolan, A. Lupan, A.M.V. Branzanic, G.L. Turdean, J. Solid Sate Electrochem., 2024, 28, 479-494; doi: 10.1007/s10008-023-05681-w
11. "Low-energy high-spin binuclear hexamethylbenzene manganese carbonyl structures with partially bonded benzene rings" M. Arpenti, A. Lupan, R.B. King, J. Organomet. Chem., 2023, 997, 122792; doi: 10.1016/j.jorganchem.2023.122792
12. "Polyhedral ferraboranes with iron carbonyl vertices: carbonyl migration processes in the iron tetracarbonyl derivatives" A.A. Attia, A. Lupan, R.B. King, J. Phys. Chem. A, 2023, 127, 5887-5898; doi: 10.1021/acs.jpca.3c02944
13. "Effect of the coordination environment on the ability of iron to bind/ activate N2: A theoretical study with relevance to the nitrogenase mechanism" R. Doukeh, D. Crăciun, A. Lupan, A.M.V. Branzanic, R. Silaghi-Dumitrescu, Polyhedron, 2023, 243, 116571; doi: 10.1016/j.poly.2023.116571
14. "Synthesis, characterisation, and in vitro cytotoxic Activity of dithiocarbamato glycoconjugate half-Sandwich Ruthenium and Osmium Complexes" J.J. Soldevila-Barreda, A. Pettenuzzo, M. Azmanova, L. Rafols, A.A. Attia, A. Lupan, L. Ronconi, N.P. Barry, A. Pitto-Barry, Helv. Chim. Acta, 2023, 106, e202300064, doi: 10.1002/hlca.202300064
15. "Polyhedral dicobaltadithiaboranes and dicobaltdiselenaboranes as examples of bimetallic nido structures without bridging hydrogens" A.A. Attia, A. Lupan, R.B. King, Molecules, 2023, 28, 2988; doi: 10.3390/molecules28072988
16. "Versatility of thiourea dioxide as redox agent in globins: case study with myoglobin" O. Rudenco, M. Lehene, A. Lupan, C. Zagrean-Tuza, B. Stoean, A. Gaina-Gardiuta, A.M. Ulici, R. Silaghi-Dumitrescu, Inorg. Chim. Acta, 2023, 551, 121474; doi: 10.1016/j.ica.2023.121474
17. "Aromaticity in P8 allotropes and (CH)8 analogues: significance of their 40 valence electrons?" A.A. Attia, A. Lupan, R.B. King, Phys. Chem. Chem. Phys., 2023, 25, 9364-9372; doi: 10.1039/d3cp00147d
18. "Triplet spin-state capped deltahedral structures rather than singlet spin-state oblatocloso structures as energetically favored dimanganaborane structures" A. Gaina-Gardiuta, A. Lupan, R.B. King, Inorg. Chem., 2022, 61, 20793-20803; doi: 10.1021/acs.inorgchem.2c02936
19. "Combining a weak-field rigid chelating bidentate dicarbene ligand with a strong-field carbonyl ligand in binuclear cyclopentadienyliron carbonyl derivatives" C. Balaiu, A. Lupan, R.B. King, Polyhedron, 2022, 219, 115778; doi: 10.1016/j.poly.2022.115778
20. "Cyclopentadienylmetal group 6 metal carbonyl derivatives with 2-propanoneoximato and related ligands" T.M. Danescu, R. Silaghi-Dumitrescu, A. Lupan, R.B. King, New J. Chem, 2021, 45, 21092-21099; doi: 10.1039/d1nj04379j
21. "Peroxo-transition metals systems: examples of redox isomerism in palladium structures" I.A. Suciu, R. A. Lupan, Silaghi-Dumitrescu, Rev. Roum. Chim, 2021, 66, 819-828; doi: 10.33224/rrch.2021.66.10-11.05
22. "Binuclear ethylenedithiolate iron carbonyls: a density functitonal theory study" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan, R.B. King, Inorg. Chim. Acta, 2021, 519, 120260; doi: 10.1016/j.ica.2021.120260
23. "Iron carbonyl complexes of a rigid chelating dicarbene: a density functional theory study" C. Balaiu, A.A. Attia, A. Lupan, R.B. King, Inorg. Chim. Acta, 2021, 514, 120002; doi: 10.1016/j.ica.2020.120002
24. "Isocloso versus closo deltahedra in slightly hypoelectronic supraicosahedral 14-vertex dimetallaboranes with 28 skeletal electrons: relationship to icosahedral dimetallaboranes" S. Jákó, A. Lupan, A.Z. Kun, R.B. King, New J. Chem., 2020, 44, 16977-16984; doi: 10.1039/d0nj03572f
25. "Enhncement of ion pairing o Sr(II) and Ba(II) salts by a tritopic ion-pair receptor in solution" B. Kutus, J. Zhu, J. Luo, Q.Q. Wang, A. Lupan, A.A. Attia, D.-X. Wang, J. Hunger, ChemPhysChem, 2020, 21, 1957-1965; doi: 10.1002/cphc.202000507
26. "Novel non-spherical deltahedra in tetramolybdaborane structures: Generation of low-energy structures by capping Mo4B4 cubes" A.A. Attia, A. Lupan, R.B. King, Polyhedron, 2020, 187, 114626; doi: 10.1016/j.poly.2020.114626
27. "The sound of Chemistry: translating infrared wavenumbers into musical notes" N. Garrido, A. Pitto-Barry, J.J. Solevila-Barreda, A. Lupan, L. Comerford Boyes, W.H.C. Martin, N.P.E. Barry, J. Chem. Educ., 2020, 97, 703-709; doi: 10.1021/acs.jchemed.9b00775
28. "Nonsphericity in diferratetracarbaboranes having 2n + 2 Wadean skeletal electrons: deviations from closo deltahedral geometries and high-energy kinetically stable isomers" A.A. Attia, A. Lupan, R.B. King, Phys. Chem. Chem. Phys., 2020, 22, 2437-2448; doi: 10.1039/c9cp04777h
29. "Neutral rhenadicarbaboranes with Re(CO)2(NO) vertices: a theoretical study of building blocks for rhenacarborane-based drug delivery agents" A.A. Attia, A. Lupan, R. Silaghi-Dumitrescu, R.B. King, Molecules, 2020, 25, 110; doi: 10.3390/molecules25010110
30. "The tetracapped truncated tetrahedron in 16-vertex tetrametallaborane structures: spherical aromaticity with an isocloso rather than a closo skeletal electron count" A.A. Attia, A. Lupan, R.B. King, S. Ghosh, Phys. Chem. Chem. Phys., 2019, 21, 22022-22030; doi: 10.1039/c9cp04263f
31. "The group 9 cyclopentadienylmetal cis Ethylenedithiolates as Metallodithiolene Ligands in Metal Carbonyl Chemistry: Analogies to Benzene Metal Carbonyl Complexes" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan, R.B. King, New J. Chem., 2019, 43, 12711-12718; doi: 10.1039/C9NJ02478F
32. "Design, synthesis and structure of novel dendritic G-2 melamines comprising piperidine motifs as key linkers and 4-(n-octyloxy)aniline as a peripheral unit" C. Sacalis, C. Morar, P. Lameiras, A. Lupan, R. Silaghi-Dumitrescu, A. Bende, G. Katona, D. Porumb, D. Harakat, E. Gal, M. Darabantu, Tetrahedron, 2019, 75, 130468; doi: 10.1016/j.tet.2019.130468
33. "Cationic gold clusters with eight valence electrons: possible spherical aromatic systems with sigma holes" A.A. Attia, A. Branzanic, A. Muñoz-Castro, A. Lupan, R.B. King, Phys. Chem. Chem. Phys., 2019, 21, 17779-17785; doi: 10.1039/C9CP03440D
34. "Versatile coordination behaviour of chloro-tetrazine-picolylamine ligand: mixed-valence binuclear Cu(I)/Cu(II) complexes" O. Stetsiuk, S. R. Petrusenko, Lorenzo Sorace, A. Lupan, A. Attia, V. Kokozay, A. El-Ghayoury, N. Avarvari, Dalton Trans., 2019, 48, 11966-11977; doi: 10.1039/C9DT02379H

35. "Magnesium(II) D-gluconate complexes relevant to radioactive waste disposals: metal ion-induced ligand deprotonation or ligand-promoted metal ion hydrolysis?" B Kutus, C. Dudás, Csilla, E. Orban, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, G. Peintler, Inorg Chem, 2019, 58, 6832-6844; doi: 10.1021/acs.inorgchem.9600289
36. "First-in-class allosteric inhibitors of bacterial IMPDHs" T. Alexandre, A. Lupan, O. Helynck, S. Vichier-Guerre, L. Dugue, M. Gelin, A. Haouz, G. Labesse, H. Munier-Lehmann, Eur. J. Med. Chem., 2019, 167, 124-132; doi: 10.1016/j.ejmech.2019.01.064
37. "The isocloso capped pentagonal bipyramid versus the closo bisdisphenoid in hypoelectronic eight-vertex metallaboranes having 16 skeletal electron" R.A. Șeptelean, A.A. Attia, A. Lupan, R.B. King, Int. J. Quant. Chem., 2019, 119, e25880; doi: 10.1002/qua.25880
38. "Calcium complexing behaviour of lactate in neutral to highly alkaline medium" Cs. Dudas, B. Kutus, E. Boszormenyi, G. Peintler, A.A. Attia, A. Lupan, Z. Kele, P. Sipos, I. Palinko, J. Mol. Struct., 2019, 1180, 491-498; doi: 10.1016/j.molstruc.2018.12.020
39. "Spherical closo deltahedra with surface metal-metal multiple bonding versus oblate deltahedra with internal metal-metal bonding in dichromadicarbaborane structures: the nature of Stone's icosahedral dichromadicarbaborane" S. Jákó, A. Lupan, A.Z. Kun, R.B. King, Inorg. Chem., 2019, 58, 3825-3837; doi: 10.1021/acs.inorgchem.8b03476
40. "Reversible complexation of ammonia by breaking a manganese-manganese bond in a manganese carbonyl ethylenedithiolate complex: A theoretical study of an unusual type of Lewis acid" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan*, R.B. King, Dalton Trans., 2019, 48, 324-332; doi: 10.1039/C8DT04217A
41. "Segregation of tetracarbon units in low-energy tetracarbindane structures: major differences from their aluminum and gallium analogues" A.A. Attia, A. Lupan, R.B. King, Int. J. Quant. Chem., 2019, 119, e25934; doi: 10.1002/qua.25934
42. "The acidity and self-catalyzed lactonization of L-gulonic acid: Thermodynamic, kinetic and computational study" B. Kutus, G. Peintler, A Bucko, Z. Balla, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, Carbohydrate Res., 2018, 467, 14-22; doi: 10.1016/j.carres.2018.07.006
43. "Opening cobaltadicarbaborane deltahedra by external dimethylamino substituents: conversion of icosahedra to isonido 12-vertex polyhedra" A.A. Attia, A. Lupan, R.B. King, Polyhedron, 2018, 151, 458-464; doi: 10.1016/j.poly.2018.06.003
44. "Binuclear pentalene titanium carbonyls: comparison with related cyclopentadienyltitanium carbonyls" L.F. Radu, A.A. Attia, A. Lupan, R.B. King, Int. J. Quant. Chem., 2018, 118, e25762; doi: 10.1002/qua.25762
45. "Polyhedral trimetallaboranes of the group 9 metals: isocloso versus capped and uncapped closo deltahedra" A.A. Attia, A. Lupan, R.B. King, Organometallics, 2018, 37, 1845-1851; doi: 10.1021/acs.organomet.8b00077
46. "New class of hybrid materials for detection, capture and on-demand release of carbon monoxide" A. Pitto-Barry, A. Lupan, C. Ellingford, A.A. Attia, N.P. Barry, ACS Appl. Mater. Interfaces, 2018, 10, 13693-13701; doi: 10.1021/acsami.8b01776
47. "Group 9 metallatelluraboranes: comparison with their sulfur analogues" A.A. Attia, A. Lupan, R.B. King, J. Organomet. Chem., 2018, 865, 145-151; doi: 10.1016/j.jorganchem.2018.01.058
48. "Major differences between preferred tetracarbagallane and tetracarbalane structures" A.A. Attia, A. Lupan, R.B. King, J. Organomet. Chem., 2018, 864, 88-96; doi: 10.1016/j.jorganchem.2018.01.051
49. "Tetracapped tetrahedral ruthenium-sulfur clusters related to iron-sulfur structural units in metalloenzymes" A. Lupan, R. Silaghi-Dumitrescu, R.B. King, Inorg. Chim. Acta, 2018, 475, 193-199; doi:10.1016/j.ica.2017.10.011
50. "Metal-metal bonding in deltahedral dimetallaboranes and trimetallaboranes: a density functional theory study" A.A. Attia, A. Lupan, R.B. King, Pure Appl. Chem., 2018, 90, 643-652; doi: 10.1515/pac-2017-0906
51. "Aluminum-poor hexacarbalane structures: the transition from localized organoaluminum structures to delocalized polyhedra" A.A. Attia, A. Lupan, R.B. King, Int. J. Quant. Chem., 2018, 118, e25506; doi: 10.1002/qua.25506
52. "Binuclear pentalene titanium carbonyls involved in the deoxygenation of carbon dioxide" L.F. Radu, A.A. Attia, A. Lupan, R.B. King, J. Organomet. Chem., 2018, 867, 201-207; doi: 10.1016/j.jorganchem.2017.11.006
53. "Deviations from the most spherical deltahedra in rhenatricarbaboranes having 2n + 2 wadean skeletal electrons" A.A. Attia, A. Lupan, R.B. King, Inorg. Chem., 2017, 56, 15015-15025; doi: 10.1021/acs.inorgchem.7b02348
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55. "Pseudo electron-deficient organometallics: limited reactivity towards electron-donating ligands" A. Pitto-Barry, A. Lupan, M. Zegke, T. Swift, A.A. Attia, R.M. Lord, N.P. Barry, Dalton Trans., 2017, 46, 15676-15683; doi: 10.1039/C7DT02827J
56. "Paramagnetism in metallacarboranes: the polyhedral chromadicarbaborane systems" S. Jákó, A. Lupan, A.Z. Kun, R.B. King, Inorg Chem, 2017, 56, 11059-11065; doi: 10.1021/acs.inorgchem.7b01422
57. "Novel non-spherical deltahedra in tritungstaboranes related to the experimentally known Cp*3W3(H)B8H8" A.A. Attia, A. Lupan, R.B. King, New J. Chem., 2017, 41, 10640-10651; doi: 10.1039/C7NJ01801K
58. "Formation of mono and binuclear neodymium(III)-gluconate complexes in aqueous solutions in the pH range of 2-8" B. Kutus, N. Varga, G. Peintler, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, Dalton Trans., 2017, 46, 6049-6058; doi: 10.1039/C7DT00909G
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62. "Metal-Metal multiple Bonds with "half-bond" components in paramagnetic organometallics of f-block metals" C. Cosar, A.A. Attia, A. Lupan, R.B. King, J. Organometal. Chem., 2017, 827, 105-111; doi: 10.1016/j.jorganchem.2016.11.006

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65. "Hydrogen migration in hypoelectronic biicosahedral metallaborane structures" A.A. Attia, A. Lupan, R.B. King, RSC Adv., 2016, 6, 87096-87102; doi: 10.1039/C6RA16304A
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