

Andrzej Sygula

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RESEARCH INTERESTS:

Organic and Physical Organic Chemistry: Polycyclic Aromatic Hydrocarbons (PAH's), including Buckybowls, *i.e.* curved-surface class of PAH's related to fullerenes; development of efficient synthetic methodologies leading to strained aromatic systems; supramolecular complexes; conformation studies by both spectroscopic and theoretical methods; molecular modeling; application of computational methods to problems of organic chemistry.

EDUCATION:

- 1985-1986 Postdoctoral Fellow; Department of Chemistry, Indiana University - Purdue University at Indianapolis, IN 46223.
Research Area: "Dissolving Metal Reduction of Polycyclic Aromatic Hydrocarbons"
Postdoctoral Advisor: Prof. Peter W. Rabideau
- 1982 Ph.D.: Organic Chemistry
Jagiellonian University, Department of Chemistry, Krakow, Poland
Dissertation Title: "Self-association of 2-Quinolones"
Major Professor: Julian Mirek
- 1976 M.S., Organic chemistry
Jagiellonian University, Department of Chemistry,
Krakow, Poland

ACADEMIC APPOINTMENTS:

- 2010-present Professor of Chemistry,
Department of Chemistry, Mississippi State University
Mississippi State, MS 39762
- Fall 2014 Visiting Professor
Department of Chemistry,
Jagiellonian University, Krakow, Poland

2003-2010 Associate Professor of Chemistry,
Department of Chemistry, Mississippi State University
Mississippi State, MS 39762

2001-2003 Associate Scientist,
Department of Chemistry and Ames Laboratory, Iowa State
University, Ames, IA 50011

1999-2001 Assistant Scientist III,
Department of Chemistry and Ames Laboratory, Iowa State
University, Ames, IA 50011

1994-1999 Assistant Professor-Research, Department of Chemistry,
Louisiana State University, Baton Rouge, LA

1990-1994 Postdoctoral Researcher, Department of Chemistry,
Louisiana State University, Baton Rouge, LA

1982-1991 Assistant Professor, Department of Chemistry,
Jagiellonian University, Krakow, Poland

1981-1982 Research and Teaching Assistant, Department of Organic
Chemistry, Jagiellonian University, Krakow, Poland

1977-1981 Graduate Student, Department of Chemistry,
Jagiellonian University, Krakow, Poland

1976-1977 Research Assistant, Department of Chemistry,
Jagiellonian University, Krakow, Poland

PROFESSIONAL AFFILIATIONS:

The American Chemical Society

SYNERGISTIC ACTIVITIES:

Serves as a peer reviewer for *Journal of the American Chemical Society*, *Journal of Organic Chemistry*, *Organic Letters*, *New Journal of Chemistry*, etc. as well as a reviewer of Grant Proposals (NSF, DOE)

Served as a Coordinator for the External Seminar Program of the Department of Chemistry, MSU

Serves on several Graduate Committees in the Department of Chemistry

Chaired the Departmental Search Committee for the Instructor position

Chaired the Departmental Promotion and Tenure Committee

AWARDS:

James W. Bagley Faculty Award (October 2011).

Arts & Sciences Faculty State Pride Award (September 2010).

Arts & Sciences Dean's Eminent Scholar Award (2009-2012).

Mississippi State University A&S Researcher of the Month (March 2009).

Jagiellonian University Chancellor's Award for Achievements in Sciences, 1988.

PUBLICATIONS:

Book Chapters:

“Molecular Clips and Tweezers with Corannulene Pincers”

Sygula, A.; Collier, W.

Chapter 1 in “*Fragments of Fullerenes and Carbon Nanotubes: Design Synthesis, Unusual Reactions, and Coordination Chemistry*”

Petrukhina, M. A.; Scott, L. T., Eds.; Wiley; Hoboken, NJ, **2011**, p 1- 40.

“Synthesis and Chemistry of Polycyclic Aromatic Hydrocarbons with Curved Surfaces: Buckybowls”

Sygula, A.; Rabideau, P. W.

Chapter 12 in “*Carbon-Rich Compounds: From Molecules to Materials*” Haley, M.; Tykwinski, R., Eds.; Wiley-VCH Publisher, Weinheim, **2006**, p 529 - 565.

"Polynuclear Aromatic Hydrocarbons with Curved Surfaces: Hydrocarbons Possessing Carbon Frameworks Related to Buckminsterfullerene"

Rabideau, P. W., Sygula, A.

In “*Advances in Theoretically Interesting Molecules*” Thummel, R. P., Ed.; JAI Press, Inc., Greenwich, CT, Vol. 3, **1995**, p 1 - 36.

"Conformational Analysis of 1,3-Cyclohexadiene and Related Hydrocarbons".

Rabideau, P.W.; Sygula, A.

In “*The Conformational Analysis of Cyclohexenes, Cyclohexadienes and Related Hydroaromatic Compounds*” Rabideau, P.W., Ed.; VCH Publisher, **1989**, p 67-89.

Refereed Publications:

92. “Corannulene-Adorned Molecular Receptors for Fullerenes Utilizing π - π Stacking of the Curved-Surface Conjugated Carbon Networks. Design, Synthesis and Testing”
Invited auto-review in Synlett Cluster Issue “Synthesis of Non-planar Polyaromatic Compounds”
Sygula, A.
SYNLETT **2016**, 27, 2070-2080.
91. “Bis-corannulenoanthracene - an Angularly Fused Pentacene as a Precursor for Barrelene-tethered Receptors for Fullerenes”
Kumarasinghe, K.G.U. R.; Fronczek, F. R.; Valle, H. U.; Sygula, A.
Org. Lett. **2016**, 18, 3054-3057.
90. “Bis-corannulene Receptors for Fullerenes Based on Klärner’s Tethers: Reaching the Affinity Limits”
Abeyratne Kuragama, P. L.; Fronczek, F. R.; Sygula, A.
Org. Lett., **2015**, 17, 5292-5295.
89. “A 2:1 Receptor/ C_{60} Complex as a Nanosized Universal Joint”
Yanney, M.; Fronczek, F. R.; Sygula, A.
Angew. Chem. Int. Ed. **2015**, 54, 11153-11156.

88. "Thermodynamics of Host-Guest Interactions Between Fullerenes and a Buckycatcher"
Le, V. H.; Yanney, M.; McGuire, M.; Sygula, A., Lewis, E. A.
J. Phys. Chem. B **2014**, *118*, 11956-11964.
87. "Inclusion Complexes and Solvates of Buckycatcher, a Versatile Molecular Host with Two Corannulene Pincers"
Sygula, A.; Yanney, M.; Henry, W. P.; Fronczek, F. R.; Zabula, A. V.; Petrukhina, M. A.
Cryst. Growth Des. **2014**, *14*, 2633-2639.
86. "Particle in a Disc: A Spectroscopic and Computational Laboratory Exercise Studying the Nanomolecular Building Block Corannulene"
Frey, E.; Sygula, A.; Hammer, N.
J. Chem. Educ., **2014**, *91*, 2186-2190.
85. "Unsolvated Buckycatcher and its First Dianion"
Zabula, A. V.; Sevryugina, Y. V.; Spisak, S. N.; Kobryn, L.; Sygula, R.; Sygula, A.; Petrukhina, M. A.
Chem. Commun. **2014**, *50*, 2657-2659.
84. "Tridental Molecular Clips with Corannulene Pincers: Is Three better than Two?"
Yanney, M., Sygula, A.
Tetrahedron Lett., **2013**, *54*, 2604-2607.
83. "Corannulene Subunit Acts as a Diene in a Cycloaddition Reaction: Synthesis of C₈₀H₃₂ Corannulyne Tetramer"
Yanney, M., Fronczek, F. R., Sygula, A.
Org. Lett. **2012**, *14*, 4941-4945.
82. "(E)-3,3',4,4',7,7',8,8'-Octamethyl-2H,2'H-1,1'-bi(cyclopenta[fg]acenaphthylidene)-2,2',5,5',6,6'-hexaone dichloromethane monosolvate"
McCandless, G. T.; Sygula, A.; Rabideau, P. W.; Watkins, S. F.; Fronczek, F. R.
Acta Cryst. **2012**, *E68*, o1458-o1459.
81. "Probing the Zero-Field Splitting in the Ordered N@C₆₀ in Buckycatcher C₆₀H₂₈ Studied by EPR Spectroscopy"
Yang, J.; Feng, P., Sygula, A.; Harneit, W.; Su, J-H.; Du, J.
Phys. Lett. A, **2012**, *376*, 1748-1751.
80. "Cyclotrimerization of Corannulyne: Steric Hindrance Tunes the Inversion Barriers of Corannulene Bowls"
Yanney, M.; Fronczek, F. R.; Henry, W. P.; Beard, D. J.; Sygula, A.
Eur. J. Org. Chem. **2011**, 6636-6639.

79. "Epirubicin-[anti-HER2/neu] Synthesized with an Epirubici-(C₁₃-imino)-EMCS Analog: Anti-Neoplastic Activity against Chemotherapeutic-Resistant SKBr-3 Mammary Carcinoma in Combination with Organic Selenium"
Coyne, C. P.; Jones, T.; Sygula, A.; Bailey, J.; Pinchuk, L.
J. Cancer Ther. **2011**, 2, 22-39.
78. "Concave-Convex Stacking of Curved Conjugated Networks: Benchmark Calculations on the Corannulene Dimer"
Janowski, T.; Pulay, P.; Karunarathna, A. A. S.; Sygula, A.; Saebo, S.
Chem. Phys. Lett. **2011**, 512, 155-160.
77. "Chemistry on a Half-Shell: Synthesis and Derivatization of Buckybowls"
Sygula, A.
Eur. J. Org. Chem. **2011**, 1611-1625.
76. "Determination of the Binding Affinity, Packing, and Conformation of Thiolate and Thione Ligands on Gold Nanoparticles"
Ansar, S. M.; Haputhanthri, R.; Edmonds, B.; Liu, D.; Yu, L.; Sygula, A.; Zhang, D. *J. Phys. Chem. C* **2011**, 115, 653-660.
75. "Acid Cleavable Surface Enhanced Raman Tagging for Protein Detection"
Zhang, D.; Vangala, K.; Li, S.; Yanney, M.; Xia, H.; Zou, S.; Sygula, A. *Analyst* **2011**, 136, 520-526.
74. "Sensitive Carbohydrate Detection Using Surface Enhanced Raman Tagging"
Vangala, K.; Yanney, M.; Hsiao, C.-T.; Wu, W. W.; Shen, R.-F.; Zou, S.; Sygula, A.; Zhang, D. *Anal. Chem.* **2010**, 82, 10164-10171.
73. "Ultrasensitive Detection of Malondialdehyde with Surface Enhanced Raman Spectroscopy" Zhang, D.; Haputhanthri, R.; Ansar, S. M.; Vangala, K.; De Silva, H. I.; Sygula, A.; Saebo, S.; Pittman C. U. Jr. *Anal. Bioanal. Chem.* **2010**, 398, 3193-3201.
72. "Inclusion Complexes of Buckycatcher with C₆₀ and C₇₀"
Mück-Lichtenfeld, C.; Grimme, S.; Kobryn, L., Sygula, A.; *Phys. Chem. Chem. Phys.* **2010**, 12, 7091-7097.
71. "Molecular Clips and Tweezers with Corannulene Pincers" Kobryn, L.; Henry, W. P.; Fronczek, F. R.; Sygula, R.; Sygula, A. *Tetrahedron Lett.* **2009**, 50, 7124-7127.
70. "Evidence for π -Stacking as a Source of Stereocontrol in the Synthesis of the Core Pyranochromene Ring System Common to Calyxin I, Calyxin J, and Epicalyxin J"
Polat Cakir, S.; Stokes, S.; Sygula, A.; Mead, K. *J. Org. Chem.* **2009**, 74, 7529-7532.
69. "Radiometric Raman Spectroscopy for Quantification of Protein Oxidative Damage" Zhang, D.; Jiang, D.; Yanney, M.; Sygula, A. *Anal. Biochem.* **2009**, 391, 121-126.
68. " π - π Stacking of Curved Carbon Networks: The Corannulene Dimer"

- Sygula, A.; Saebo, S.
Int. J. Quant. Chem. **2009**, *109*, 65-72.
67. “2-Trimethylsilylcorannulenyl Trifluoromethanesulfonate: An Efficient Precursor for 1,2-Didehydrocorannulene”
Sygula, A.; Sygula, R.; Kobryn, L.
Org. Lett., **2008**, *10*, 3927-3929.
66. “A Double Concave Hydrocarbon Buckycatcher”
Sygula, A.; Fronczek, F. R.; Sygula, R.; Rabideau, P. W.; Olmstead, M. M.
J. Am. Chem. Soc. **2007**, *129*, 3842-3843.
65. “ η^6 -Coordination of the Curved Carbon Surface of Corannulene (C₂₀H₁₀) to (η^6 -arene)M²⁺ (M = Ru, Os)”
Zhu, B.; Ellern, A.; Sygula, A.; Sygula, R.; Angelici, R. J.
Organometallics **2007**, *26*, 1721-1728.
64. “Isocorannulenofuran: A Versatile Building Block for the Synthesis of Large Buckybowls”
Sygula, A.; Sygula, R.; Rabideau, P. W.
Org. Lett. **2006**, *8*, 5909-5911.
63. “The First Buckybowl Aryne: Corannulyne – a Nonplanar Benzyne”
Sygula, A.; Sygula, R.; Rabideau, P. W.
Org. Lett. **2005**, *7*, 4999-5001.
62. “Flattening of a Curved-Surface Buckybowl (Corannulene) by η^6 -Coordination to {Cp*Ru}⁺”
Vecchi, P. A.; Alvarez, C. M.; Ellern, A.; Angelici, R. J.; Sygula, A.; Sygula, R.; Rabideau, P. W.
Organometallics, **2005**, *24*, 4543-4552.
61. “Barrelene-Semibullvalene Rearrangement Induced by Visible Light: Synthesis of Dicarannulenosemibullvalene Dimethyl Dicarboxylate”
Sygula, A.; Sygula, R.; Rabideau, P. W.
Tetrahedron Lett. **2005**, *46*, 1189-1192.
60. “Synthesis and Structure of Dimetallated Buckybowl: Coordination of One [Cp*Ru]⁺ Unit to Each Side of Corannulene”
Vecchi, P. A.; Alvarez, C. M.; Ellern, A.; Angelici, R. J.; Sygula, A.; Sygula, R.; Rabideau, P. W.;
Angew. Chem. Int. Ed. **2004**, *43*, 4497-4500.
59. “Novel Twin Corannulene: Synthesis and Crystal Structure Determination of Dicarannulenobarrelene”
Sygula, A.; Sygula, R. Ellern, A.; Rabideau, P. W.
Org. Lett. **2003**, *5*, 2595-2597.

58. "Hexahapto Corannulene Buckybowl Complexes of Iridium, Including Ring-to-Ring Migration"
Alvarez, C. M.; Angelici, R. J.; Sygula, A.; Sygula, R.; Rabideau, P. W.
Organometallics, **2003**, *22*, 624-626.
57. "Improved Synthesis of Benz[*a*]acephenanthrene"
Marcinow, Z.; Sygula, A.; Rabideau, P. W.
Synlett. **2002**, 1839-1840.
56. "Formation of the Corannulene Core by Nickel-Mediated Intramolecular Coupling of Benzyl and Benzylidene Bromides: A Versatile Synthesis of Dimethyl 1,2-Corannulene Dicarboxylate"
Sygula, A.; Karlen, S. D.; Sygula, R.; Rabideau, P. W.
Org. Lett. **2002**, *4*, 3135-3137.
55. "The Addition of Organolithium Reagents to Corannulene and Conformational Preferences in 1-Alkyl-1,2-Dihydrocorannulenes"
Sygula, A.; Sygula, R.; Fronczek, F. R.; Rabideau, P. W.
J. Org. Chem. **2002**, *67*, 6487-6492.
54. "Lowering Inversion Barriers of Buckybowls by Benzannelation of the Rim: Synthesis and Crystal and Molecular Structure of 1,2-Dihydrocyclopenta[*b,c*]dibenzo[*g,m*]corannulene"
Marcinow, Z.; Sygula, A.; Ellern, A.; Rabideau, P. W.
Org. Lett. **2001**, *3*, 3527-3529.
53. "Buckybowls – Introducing Curvature by Solution Phase Synthesis"
Sygula, A.; Xu, G.; Marcinow, Z.; Rabideau, P. W.
Tetrahedron, **2001**, *57*, 3637-3644.
52. "The First Crystal Structure Characterization of a Semibuckminsterfullerene and a Novel Synthetic Route"
Sygula, A.; Marcinow, Z.; Fronczek, F. R.; Guzei, I.; Rabideau, P. W.
Chem. Commun., **2000**, 2439-2440.
51. "Chemistry on the Rim of Buckybowls: Derivatization of 1,2,5,6-Tetrabromocorannulene"
G. Xu,; Sygula, A.; Marcinow, Z.; Rabideau, P. W.
Tetrahedron Lett. **2000**, *41*, 9931-9934.
50. "A Simple, Large-Scale Synthesis of the Corannulene System"
Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **2000**, *122*, 6323-6624.
49. "Non-Pyrolytic Syntheses of Buckybowls: Corannulene, Cyclopentacorannulene, and a Semibuckminsterfullerene"

- Sygula, A., Rabideau, P. W.
J. Am. Chem. Soc. **1999**, *121*, 7800.
48. "Enzymatic and Nonenzymatic Production of Free Radicals from the Carcinogens 4-Nitroquinoline N-Oxide and 4-Hydroxyaminoquinoline N-Oxide"
Fann, Y. C.; Metosh-Diskey, C. A.; Winston, G. W.; Sygula, A.; Rao, D. N. R.; Kadiiska, M. B.; Mason, R. P.
Chem. Res. Toxicol. **1999**, *12*, 450.
47. "The First Non-Pyrolytic Synthesis of a Semibuckminsterfullerene"
Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **1998**, *120*, 12666.
46. "The First Crystallographically Characterized Transition Metal Buckybowl Compound: C₃₀H₁₂ Carbon-Carbon Bond Activation by Pt(PPh₃)₂"
Shaltout, R. M.; Sygula, R.; Sygula, A.; Fronczek, F. R.; Stanley, G. G.; Rabideau, P. W.
J. Am. Chem. Soc. **1998**, *120*, 835.
45. "Fullerene Fragments: Synthesis and Crystal Structure Determination of 1,4,5,6,7,10,11,12-Octamethylindeno[1,2,3-*cd*]fluoranthene"
Sygula, A., Fronczek, F. R., Rabideau, P. W.
Tetrahedron Lett. **1997**, *38*, 5095.
44. "The First Example of η^8 Coordination of the Lithium Cations with the Cyclooctatetrenyl Anion: Crystal Structure of Li₂(dibenzo[*a,e*] cyclooctatetraene)(TMEDA)₂"
Sygula, A., Fronczek, F. R., Rabideau, P. W.
J. Organomet. Chem. **1996**, *526*, 389.
43. "Investigations of Dehydroepiandrosterone. Part I: Crystal Structure of Sublimed DHEA"
Bhacca, N. S., Fronczek, F. R., Sygula, A.
J. Chem. Cryst. **1996**, *26*, 483.
42. "Buckybowls: Polynuclear Aromatic Hydrocarbons Related to the Buckminsterfullerene Surface"
Rabideau, P. W., Sygula, A.
Acc. Chem. Res. **1996**, *29*, 235.
41. "Cyclopentacorannulene: π -Facial Stereoselective Deuterogenation and Determination of the Bowl-to-Bowl Inversion Barrier for a Constrained Buckybowl"
Sygula, A.; Abdourazak, A. H.; Rabideau, P. W.
J. Am. Chem. Soc. **1996**, *118*, 339.
40. "Buckybowls II. Towards the Total Synthesis of Buckminsterfullerene (C₆₀): Benz[5,6]-*as*-indaceno[3,2,1,8,7-*mno*qr]indeno[4,3,2,1-*cdef*]chrysene"
Abdourazak, A. H.; Marcinow, Z.; Sygula, A.; Sygula, R.; Rabideau, P. W.

- J. Am. Chem. Soc.* **1995**, *117*, 6410.
39. "Structure and Inversion Barriers of Corannulene, its Dianion and Tetraanion. An *Ab Initio* Study"
Sygula, A.; Rabideau, P. W.
J. Mol. Struct. (Theochem), **1995**, *333*, 215.
38. "Buckybowls: Synthesis and Ab Initio Calculated Structure of the First Semibuckminsterfullerene"
Rabideau, P. W.; Abdourazak, A. H.; Folsom, H. E.; Marcinow, Z.; Sygula, A.; Sygula, R.
J. Am. Chem. Soc. **1994**, *116*, 7891.
37. "The First Example of Bowl Stacking in Convex Hydrocarbons: Crystal and Molecular Structure of Cyclopentacorannulene"
Sygula, A.; Folsom, H. E.; Sygula, R.; Abdourazak, A. H.; Marcinow, Z.; Fronczek, F. R.;
Rabideau, P. W.
J. Chem. Soc., Chem. Commun. **1994**, 2571.
36. "Convex vs. Concave π -Facial Binding of Metal Cations to a Semibuckminsterfullerene: An *Ab Initio* Study"
Sygula, A.; Rabideau, P. W.
J. Chem. Soc., Chem. Commun. **1994**, 2271.
35. "Stable High-Order Molecular Sandwiches: Hydrocarbon Polyanion Pairs with Multiple Lithium Inside and Out"
Ayalon, A.; Sygula, A.; Cheng, P. C.; Rabinowitz, M.; Rabideau, P. W.; Scott, L. T.
Science, **1994**, *265*, 1065.
34. "1,2,5,6-Tetraketopyracene: Synthesis and Structure by ab initio Calculations and X-ray Analysis"
Abdourazak, A. H.; Marcinow, Z.; Folsom, H. E.; Fronczek, F. R.; Sygula, R.; Sygula, A.;
Rabideau, P. W.
Tetrahedron Lett. **1994**, *35*, 3857.
33. "Bowl-to-Bowl Inversion in Polynuclear Aromatic Hydrocarbons with Curved Surfaces: An *Ab Initio* Study"
Sygula, A.; Rabideau, P. W.
J. Chem. Soc., Chem. Commun. **1994**, 1497.
32. "The Preferred U-Conformation of *m*-Quinquephenyl. An X-Ray Crystal Structure Determination and Molecular Mechanics Study"
Rabideau, P. W.; Sygula, A.; Dhar, R. K.; Fronczek, F. R.
J. Chem. Soc., Chem. Commun. **1993**, 1795.
31. "Concerning the Structure of the Corannulene Tetraanion"
Rabideau, P. W.; Marcinow, Z.; Sygula, R.; Sygula, A.
Tetrahedron Lett. **1993**, *34*, 6351.

30. "“Locking” the Bowl-Shaped Geometry of Corannulene: Cyclopentacorannulene”
Abdourazak, A. H.; Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **1993**, *115*, 3010.
29. "Ab Initio Study of the Structure and the Inversion Barriers in 1,3-Cyclohexadiene, 1,2-Dihydronaphthalene and 9,10-Dihydrophenanthrene"
Sygula, A.; Rabideau, P. W.
J. Mol. Struct., THEOCHEM, **1992**, *262*, 117.
28. "An Investigation of Substituent Effects on the Conformation of 9,10-Dihydroanthracenes by Molecular Mechanics Calculations and X-ray Structure Analysis”
Dhar, R. K.; Sygula, A.; Fronczek, F. R.; Rabideau, P. W.
Tetrahedron, **1992**, *48*, 9417.
27. "Crystal and Molecular Structure of 10-Substituted-9-Anthracenones. Substituent Size as the Controlling Factor for the Nonplanarity of the Central Ring"
Sygula, A.; Sygula, R.; Fronczek, F. R.; Rabideau, P. W.
J. Org. Chem. **1992**, *57*, 3286.
26. "Pathways for Ring Inversion in 9,10-Dihydroanthracene, 9,10-Dihydrophenanthrene and 7,12-Dihydropleiadene. A Combined Molecular Orbital and Molecular Mechanics Study."
Sygula, A.; Rabideau, P. W.
J. Comp. Chem. **1992**, *13*, 633.
25. "An Ab Initio Study of the Structure of Monomeric, Unsolvated Benzylolithium. Is Covalency of the Carbon-Lithium Bond Important?"
Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **1992**, *114*, 821.
24. "The Existence of Carbanion Triplet Structures As Evidenced by NMR Spectroscopy and MNDO/AM1 Calculations”
Sethson, I.; Johnels, D.; Lejon, T.; Edlund, U.; Wind, B.; Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **1992**, *114*, 953.
23. "The Effect of Phenyl Substitution on the Structure of Benzylic Anions"
Rabideau, P. W.; Wind, B. K.; Sygula, A.
Tetrahedron Lett. **1991**, *32*, 5659.
22. "The Structure of Dilithiobenzenide: An ab Initio Study."
Sygula, A.; Rabideau, P. W.
J. Am. Chem. Soc. **1991**, *113*, 7797.
21. "The Structure of 7,12-Dilithio-7,12-Dihydropleiadene: An Investigation by ^{13}C NMR Spectroscopy and MNDO Calculations"
Wind, B.; Sygula, A.; Govindarajan, U.; Edlund, U.; Stethson, I.; Rabideau, P. W.

- J. Org. Chem.* **1991**, *56*, 618.
20. "Electronic and Ring Current Structure of Phenalenyl Ions"
Stethson, I.; Edlund, U.; Johnels, D.; Sygula, A.
J. Chem. Soc., Perkin Tr. 2, **1990**, 1339.
 19. "A Fast and Accurate Estimation of Amide-Iminol Tautomerization Energies by the AM1 Method"
Sygula, A.
J. Chem. Res. (S), **1989**, 56.
 18. "Proton and Carbon-13 NMR Reinvestigation of the Dibenzo[a,c]cyclononatetraenyl Anion and its 5,9-Diphenyl Derivative. Planarity vs. Nonplanarity"
Eliasson, B., Nouri-Sorkhabi, M.H.; Trogen, L.; Stethson, I.; Edlund, U., Sygula, A., Rabinovitz, M.
J. Org. Chem. **1989**, *54*, 171.
 17. "A Novel Synthesis of 1,3-Thiazetid-2-one and 1,3-Oxazin-2-one Derivatives"
Zankowska-Jasinska, W.; Burgiel, M.; Danel, A., Sygula, A.
J. Prakt. Chem. **1988**, *330*, 795.
 16. "Metal-ammonia Reduction of Triphenylene"
Marcinow, Z.; Sygula, A.; Rabideau, P.W.
J. Org. Chem. **1988**, *53*, 3603.
 15. "Dissolving Metal Reduction of Aceanthrylene and NMR Analysis of a Rigid, Boat-Shaped 9,10-Dihydroanthracene"
Rabideau, P.W.; Mooney, J.L.; Smith, W.K.; Sygula, A.; Paschal, J.W.
J. Org. Chem. **1988**, *53*, 589.
 14. "Structure of the Cyclononatetraenyl Anion and Some of Its Benzannulated Derivatives. A Semiempirical MNDO and AM1 Study"
Sygula, A.; Edlund, U.; Rabideau, P.W.
J. Chem. Res. (S), **1987**, 312.
 13. "Nature of Carbon-Lithium Bonding in Dilithiated Polynuclear Aromatics: An MNDO Study"
Sygula, A.; Lipkowitz, K.; Rabideau, P.W.
J. Am. Chem. Soc. **1987**, *109*, 6602.
 12. "Structure of 9-Substituted 9,10-Dihydroanthracene Monoanions. A Semiempirical MO Study"
Sygula, A.; Rabideau, P.W.
J. Org. Chem. **1987**, *52*, 3521.
 11. "On the Possibility of Fluorescence from Twisted Intramolecular Charge Transfer States of 2-Dimethylamino-6-Acylnaphthalenes. A Quantum-Chemical Study"

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 7. "Carbon-13 Proton Coupling Constants in 9,10-Dihydroanthracene"
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 5. "MNDO Study of the Tautomers of Nucleic Bases. Part I. Uracil, Thymine and Cytosine"
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 3. "MNDO Studies on Relative Stabilities of Monosubstituted Pyridine Tautomers"
Mirek, J.; Sygula, A.
J. Mol. Struct. THEOCHEM, **1981**, 3, 85.
 2. "Self-Association of 4-Methyl-2-Quinolone"
Mirek, J.; Sygula, A.
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 1. "An (α - ϵ) Proximity Interaction Between Oxime Hydroxyl and α -Protons of 1-Indanone Oxime"
Mirek, J.; Oglaza, L.; Sygula, A.
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NEWS ARTICLES AND NOTES:

A number of news articles and notes have appeared featuring some of the above publications:

Publication No. 87

“Crystal Structure Highlights Buckycatcher’s Flexibility” RCS in their ChemistryWorld, The RCS blog , January 30, **2014**

Publication No. 78 was selected as an Editor’s Choice in *Chem. Phys. Lett.* (**2011**)

Publication No. 65

“The Buckycatcher” *Nature*, News of the Week, March 22, **2007**

“Dual Buckybowl Buckycatcher” *Chemical and Engineering News*, Science and Technology Concentrates, March 26, **2007**

“Buckybowl: A Good Catch” *Nature Nanotechnology*, March 23, **2007**

Publication No. 50 & 53

“Buckybowls by the Bucketful” *U.S. Department of Energy, Office of Science Home Page*, April 28, **2001**.

“Buckybowls by the Bucketful” *USA Today*, June 1, **2001**, p.12.

“From Buckyballs to Buckybowls” *Microelectronic Technology Alert*, April 13, **2001**. Electronic publication, Frost & Sullivan, Inc.

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“Solution-Phase Route to Half of a Buckyball” *Chemical and Engineering News*, Science and Technology Concentrates, December 14, **1998**.

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“Metal-Buckybowl Structure Dishes Out a Surprise” *Chemical and Engineering News*, Science and Technology Concentrates, February 2, **1998**.

Publication No. 40

“Buckybowl Representing Half of a C₆₀ Molecule Synthesized” *Chemical and Engineering News*, Science and Technology Concentrates, June 19, **1995**.

“Fullerenes on the Half Shell” *Science*, July 21, **1995**.

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“Buckybowl – Half of a C₆₀ molecule – Synthesized” *Chemical and Engineering News*, Science and Technology Concentrates, August 29, **1994**.

“LSU Scientists Form First Buckybowls”; *ER News*, Office of Energy Research, August **1994**.

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“Corannulene Anions, Lithium Cations Form Molecular Sandwiches” *Chemical and Engineering News*, Science and Technology Concentrates, August 22, **1994**.

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“Researchers “Lock” Bowl-Shaped Geometry of Corannulene” *Chemical and Engineering News*, Science and Technology Concentrates, April 19, **1993**.

PRESENTATIONS:

“Buckybowls: Synthesis and Supramolecular Chemistry of Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

Sygula, A.

Department of Chemistry

Warsaw University

Warsaw, Poland, November 24, **2014**

“Buckybowls: Synthesis and Supramolecular Chemistry of Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

Sygula, A.

Polish Chemical Society (PTChem)

Krakow, Poland, November 19, **2014**

“Modern History of Carbon: Esthetical Chemistry?”

Sygula, A.

Third-Age University

Olkusz, Poland, November 13, **2014**

“Buckybowls: Synthesis and Supramolecular Chemistry of Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

Sygula, A.

Malopolska Centre of Biotechnology

Krakow, Poland, November 6, **2014**

“Molecular receptors for fullerenes: A buckycatcher with potential”

M. Yanney, Frank R. Fronczek, A. Sygula

2014 Southwestern Regional Meeting of ACS (SERMACS)

Nashville, TN

October 18, **2014**

“Molecular Clips and Tweezers with Corannulene Pincers on Klärner's Tethers”

P. L. Abeyratne, A. Sygula

2014 Southwestern Regional Meeting of ACS (SERMACS)

Nashville, TN

October 18, **2014**

“Buckybowls: Synthesis and Supramolecular Chemistry of Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

Sygula, A.

Department of Chemistry

University of Wroclaw

Wroclaw, Poland, October 13, **2014**

“A Perfect Catch: Engineering the Tether of the Molecular Receptors with Corannulene Pincers”

Sygula, A.

Invited Speaker, 14th Southern School on Computational Chemistry and Material Science

Jackson, MS, July 24-25, **2014**

“Buckycatcher with nothing to catch and its first reduction study”

Zabala, A. V.; Spisak, S. N.; Sevryugina, Y.; Kobryn, L.; Sygula, R.; Sygula, A.;

Petrukhina, M. A.

247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20,

2014

“Molecular Receptors for Fullerenes with Corannulene Pincers: Design, Synthesis and Performance”

A. Sygula

15th International Symposium on Novel Aromatic Compounds

Taipei, Taiwan

July 28 - August 2, **2013**.

“Molecular Clips and Tweezers with Bowl-Shaped Pincers”

A. Sygula

Department of Chemistry, Jackson State University, Jackson, MS

February 10, **2012**.

“Molecular Receptors for Fullerenes”

A. Sygula

76th Annual Meeting of Mississippi Academy of Sciences

Hattiesburg, MS

February 23, **2012**.

“Supramolecular Chemistry of Curved Surface Molecular Receptors”

68th Southwest Regional Meeting of ACS

A. Sygula

Baton Rouge, LA

November 4-7, **2012**.

“Molecular Receptors for Fullerenes: Synthesis and Characterization of a Molecular Clip with Three Corannulene Pincers”

M. Yanney, A. Sygula

68th Southwest Regional Meeting of ACS
Baton Rouge, LA
November 4-7, **2012**.

“Molecular Clips Based on the Klärner’s Tether”
P. Abeyratne, A. Sygula
68th Southwest Regional Meeting of ACS
Baton Rouge, LA
November 4-7, **2012**.

“Playing Molecular Baseball: Buckyballs and Nanoscale Catcher’s Mitts”
A. Sygula
Department of Chemistry and Biochemistry, Mississippi College, Clinton, MS
November 14, **2011**.

“Buckytriplet: Cyclotrimerization of Corannulyne”
M. Yanney, A. Sygula, F. R. Fronczek, W. P. Henry, D. J. Beard,
Joint 46th Midwest and 39th Great Lakes Regional Meeting of ACS,
St. Louis, MS,
October 19-21, **2011**.

“Concave-Convex Stacking of Curved Surface Networks: Corannulene Dimer”
A. Sygula,
11th Southern School of Computational Chemistry and Material Science
Jackson, MS, July 28, **2011**.

“Molecular Clips with Bowl-Shaped Pincers: Buckycatcher”
A. Sygula,
10th Southern School of Computational Chemistry and Material Science
Jackson, MS, April 24, **2010**.

“Polycyclic Aromatic Hydrocarbons with Curved Surfaces: Buckybowls”
A. Sygula,
“Frontiers in Organometallic and Bioinspired Catalysis Science”
DOE/BES Contractors Meeting
Annapolis, MD
June 1-4, **2010**.

“Acid Cleavable Surface Enhanced Raman Tagging for Biomolecule Detection”
K. Vangala, M. Yanney, A. Sygula, D. Zhang
Joint 66th Southwest and 62nd Southeast Regional Meeting of the American Chemical
Society, New Orleans, LA, United States, December 1-4 , **2010**.

“Toward Multimode Carbohydrate Characterization using Surface Enhanced Raman
Tagging”
D. Zhang, K. Vangala, M. Yanney, A. Sygula

Joint 66th Southwest and 62nd Southeast Regional Meeting of the American Chemical Society, New Orleans, LA, United States, December 1-4 , **2010**.

“Determination of Ligand Conformation on Gold Nanoparticle using Quantitative Surface Enhanced Raman Spectroscopy”

S. M. Ansar, R. Haputhanthri, B. Edmonds, A. Sygula, D. Zhang

Joint 66th Southwest and 62nd Southeast Regional Meeting of the American Chemical Society, New Orleans, LA, United States, December 1-4 , **2010**.

“Studies of π - π Interactions Using Density Functional Methods”

S. N. Karunarithna, A. Sygula, S. Saebo

Joint 66th Southwest and 62nd Southeast Regional Meeting of the American Chemical Society, New Orleans, LA, United States, December 1-4 , **2010**.

“Studies of π - π Interactions using Density Functional Methods”

A. A. S. Karunarithna, A. Sygula and S. Saebo

18th Conference on Current Trends in Computational Chemistry
Jackson, MS, November 30, **2009**.

“Ratiometric Raman Spectroscopy of Protein Oxidative Damage”

D. Zhang, S. Zou, A. Sygula

238th ACS National Meeting, Washington, DC, United States, August 16-20, **2009**.

“Isocorannulenofuran as a Synthone for Synthesis of New Buckybowls”

L. Kobryn, W. P. Henry and A. Sygula

SERMACS, Nashville, TN, November 12-15, **2008**.

"Assessment of Binding Energies of Molecular Clips with Fullerenes by Molecular Mechanics Calculations"

H. Beasley and A. Sygula

SERMACS, Nashville, TN, November 12-15, **2008**.

“Molecular Clips and Tweezers with Corannulene Pincers”

A. Sygula

Symposium “Fullerene Fragments and Carbon Nanotube”

ACS National Meeting

Philadelphia, PA, August 18, **2008**.

“Polycyclic Aromatic Hydrocarbons with Curved Surfaces: Buckybowls”

A. Sygula, L. Kobryn, R. Sygula, P. W. Rabideau

Meeting of the DOE/BES Catalysis and Chemical Transformations Program

Annapolis, MD

May 18-21, **2008**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

A. Sygula

Department of Chemistry, University of Alabama in Huntsville, Huntsville, AL
September 14, **2007**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

A. Sygula

Department of Chemistry, Kansas State University, Manhattan, KS
September 21, **2006**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

A. Sygula

Department of Chemistry, University of Wroclaw, Poland
June 24, **2006**

“Polycyclic Aromatic Hydrocarbons with Curved Surfaces: Buckybowls”

A. Sygula, P. W. Rabideau

Meeting of the DOE/BES Catalysis and Chemical Transformations Program
Cambridge, MD
May 21-24, **2006**

“Molecular Clips and Tweezers with Curved-Surface Corannulene Subunits”

A. Sygula

Southern School of Computational Chemistry, Jackson, MS
April 8, **2006**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

A. Sygula

Department of Chemistry, Vanderbilt University, Nashville, TN
April 3, **2006**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

A. Sygula

Materials Campus Group Luncheon, Hand Hall
Jan. 25, **2006**

“Buckybowls - Polycyclic Aromatic Hydrocarbons with Curved Surfaces”

Sygula, A.

Jackson State University, Jackson, MS, Sept. 16, **2005**

“ η^6 Complexation of $[\text{RuCp}^*]^+$ to Corannulene: Making a Plate from a Bowl”

A. Sygula, P. A. Vecchi, A. Ellern, R. J. Angelici, R. Sygula, P. W. Rabideau

11th International Symposium on Novel Aromatic Compounds (ISNA-11)
St. John's, NL, Canada; August 14-18, **2005**

“Transition metal Complexes of Buckybowls: Theory vs. Experiment”

Sygula, A.
5th Southern School of Computational Chemistry
Jackson, MS; April 8, **2005**.

“Dimetallated Buckybowl: Coordination of {Cp*Ru}⁺ to Both Sides of Corannulene”
Ellern, A.; Vecchi, P. A.; Alvarez, M. Angelici, R. J.; Sygula, A.; Sygula, R.; Rabideau,
P. W.
German Crystallographic Society Conference
Koeln, Germany, November **2004**.

“Buckybowls: Polycyclic Aromatic Hydrocarbons with Curved Surfaces”
Rabideau, P. W.; Sygula, A.
DOE Catalysis and Chemical Transformations Contractors’ Meeting
Rockville, MD, May 23-26, **2004**

“Buckyballs, Buckybowls and Graduate Studies at MSU”
Sygula, A.
Delta State University, Cleveland, MS, March 1, **2004**.

“High-yield, Non-Pyrolytic Synthesis of Corannulene”
Sygula, A.; Rabideau, P. W.
ACS National Meeting, New Orleans, LA, August **1999**.

“Buckybowls: Chemistry on a Half-Shell”
Sygula, A.
Umeå University, Umeå, Sweden, December, **1996**.

"Structure of Lithiated Polyaromatics"
Sygula, A.
Umeå University, Umeå, Sweden, May, **1988**.

“The Nature of 9-Substituted 9,10-Dihydroanthracene Monoanions”
Sygula, A.; Maxwell, A. J.; Rabideau, P. W.
ACS National Meeting, Chicago, Ill., August **1986**.

AWARDED PROPOSALS:

“Molecular Clips and Tweezers with Corannulene Pincers: Fundamental
Studies and Possibilities for Applications”
Henry Family Research Fund;
May 2016 – Dec. 2016; \$7,000.00

“Polycyclic Aromatic Hydrocarbons with Curved Surfaces: Buckybowls”
U. S. Department of Energy, Basic Energy Sciences
Feb. 2012 –Jan. 2015, \$420,000.00

Feb. 2009 – Jan. 2012, \$405,000.00
Feb. 2007 - Jan. 2009, \$250,000.00
Feb. 2004 – Jan. 2007, \$300,000.00