

C₃ News



Volume 26, Issue 1

Winter, 2001

Newsletter of College Chemistry Canada/La Chemie Collégiale au Canada



President's Report

Bob Perkins

Here we are in 2001!! It is January 4th and I am busily getting handouts ready for my first organic class on January 8th. I trust that you all had a

restful break and are ready once again to face those eager young minds in your classes. Hopefully those of you planning to travel to Montreal for the CSC/C₃ joint chemical education effort have started making your travel plans. By the time that you are reading this, the deadline for the submission of papers will have passed; hopefully your proposal was received in time. In this issue of C₃ News you will find additional details regarding the conference. Gary Wilson and Shahid Jalil have been busily getting the social events in order; I predict that a great time will be had by all.

All the best for a great finish to the semester and I hope to see many of you in Montreal at the end of May.

Bob Perkins—President

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28th College Chemistry Canada Conference and the 84th CSC Conference and Exhibition, May 26-30, 2001, Montreal

The 28th C₃ Conference will be hosted by John Abbott College and held jointly with the 84th Canadian Society for Chemistry Conference and Exhibition (ChemEd Division) at the Hilton Montreal Bonaventure Hotel in downtown Montreal, May 26 to 30, 2001. If you are attending as a C₃ member you no doubt by now will have registered with C₃ as an affiliate member, which lets you register for the conference with the CSC at the reduced rate of \$50.00. The **CSC registration form** is available at the CSC web site (listed on the C₃ web site: www.c3.douglas.bc.ca), and **the deadline for the low rate registration cost is April 30th.**

Registration for the C₃ portion of the conference is separate and a C₃ registration form needs to be submitted to Garry Wilson at John Abbott College, as there are C₃ related events that need to be registered for. No doubt many of you who are planning to attend



The much photographed Town Hall in Baie D'Urfe, near the the location of the C₃ banquet site at Fritz Farm

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the conference have already submitted a registration form, but just in case, a copy of the registration form for the C3 conference events is included with this issue of C3 News.

Accommodation details are available at the CSC web site, with a choice of various hotel accommodations or low cost accommodations at the McGill student residences.

Conference Program

There are a total of 41 submitted papers and 8 posters in the Chemical Education Division at the conference. The Chemical Education/College Chemistry Canada symposia are as follows:

Sunday AM and Sunday PM: Teaching Chemistry to Non-Chemistry Students and Explaining it to the General Public (5 papers).

Monday AM and Monday PM: How do I do it? - Experiments and Demonstrations for Introductory Chemistry Courses (9 papers)

Tuesday AM: Chemistry Teaching Laboratories for the New Millenium: Changes and Challenges - Advanced Level Laboratories (11 papers)

Tuesday PM: General Session (8 papers), Poster and Exam Question Exchange (8 posters)

Wednesday AM: Role of the TA in Chemistry Teaching (10 papers)

Wednesday PM: History of the Pharmaceutical Industry in Canada (4 papers)

Detailed abstracts for the individual submitted papers and posters, along with room locations, can be found at the CSC web site.

Conferences Events Specific to C3

Saturday May 26th 2:00 – 4:00 **c3 Executive and Board Meeting**

Sunday May 27th 6:30 am: **Annual C3 Fun Run, Mount Royal**

Monday May 28th 4:20-5:00: **C3 Annual General Meeting**

Monday May 28th 6:00 – **C3 Conference Banquet and Awards**

Presentation at Fritz Farm in Baie D'Urfe

Thursday May 31st: **C3 Tour of Mount Royal and Old Montreal**

The C3 conference banquet will be located in the very picturesque town of Baie D'Urfe at Fritz Farm. Baie D'Urfe is located near the western tip of the Island of Montreal along the north shore of Lac Saint-Louis, Lac Saint-Louis is a widening of the St. Lawrence River and John Abbott College, the host of this years social events is within walking distance. Bus transportation will be provided for those going to this banquet from the conference site. From the photograph of Fritz Farm on the next page, the site for our banquet looks very inviting! C3 will have the use of the building for the evening. The photos were kindly provided by Gary Willson of John Abbott College.

The C3 banquet will feature the annual presentation of the following awards:

- C3 Award in Chemical Education
- C3 Host College Student Scholarship
- The Chemmys
- The Fun Run Trophy
- C3 Editor's Award

It sounds like Montreal is going to be a great conference, I hope to see many of you there!

Editor

Fritz Farm, located on a large tract of land beside Lac Saint-Louis. Fritz Farm will be the site of the C3 banquet.

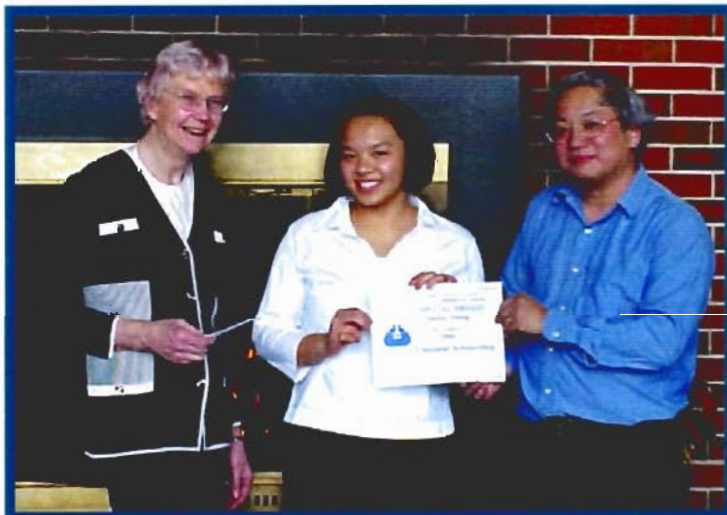


STUDENTS RECEIVE C3 SCHOLARSHIPS

This academic year C3 has awarded two General Student Scholarships. In the left hand photo is **Mirabell Eboka**, who is shown receiving her scholarship from Henry Carter and John Olson at Augustana University College. **Stella Dang** is shown receiving the 2000 C3 Student Scholarship in the right hand photo. Stella took her first year at Keyano College, and is now in second year Chemistry at the University of Alberta. The presentation was made in the U of A Faculty Club by the Assistant Chair of Chemistry, Margaret-Ann Armour, and Norman Gee, our C3 member in the Chemistry Department: It was their excellent idea to mark the occasion by taking Stella to lunch at the Faculty Club for the presentation, and everyone had a great time. Details for nominating students for this award can be found on the C3 web site.



Mirabell Eboka being presented with her C3 Student Scholarship by Henry Carter (right) and John Olson (centre). Mirabell is a student at Augustana University College in Camrose Alberta. (photo by Dan Jensen, The Camrose Booster)



Stella Dang is in second year chemistry at the University of Alberta after transferring from Keyano College. Surrounding her in the picture are Margaret-Ann Armour, Assistant Chair of Chemistry at the U of A, and Norman Gee, our C3 member on the U. of A. faculty.

Hands On Isomers - Part 2

Constitutional Isomers

Bob Perkins

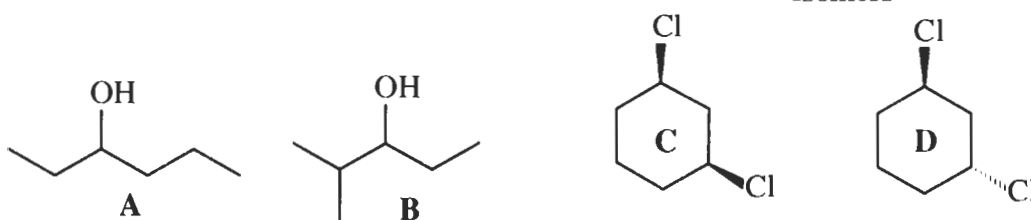
Presented in part at the 83rd Canadian Society for Chemistry Conference and Exhibition, May 27-31, 2000 at Calgary Alberta

In Part 1 of this series I described how I allow my students to have access to a summary sheet of the IUPAC prefixes and suffixes on all midterm and final exams. Once they have become proficient at recognizing functional groups and providing IUPAC names for compounds, it is now time to move on to determining the exact relationship between two isomeric compounds. There are several different classification schemes to be found in the various textbooks on the market; however, my scheme is shown below based upon the students asking themselves a series of questions when faced with compounds which have the same molecular formula.

The first question is: Do the two compounds have the same IUPAC name?

If the answer is **YES**, then the compounds are **stereoisomers** of each other. If the answer is **NO**, then the compounds are **constitutional isomers** of each other. The older term structural isomers used to be used.

I will consider the question as it applies to the following compounds.

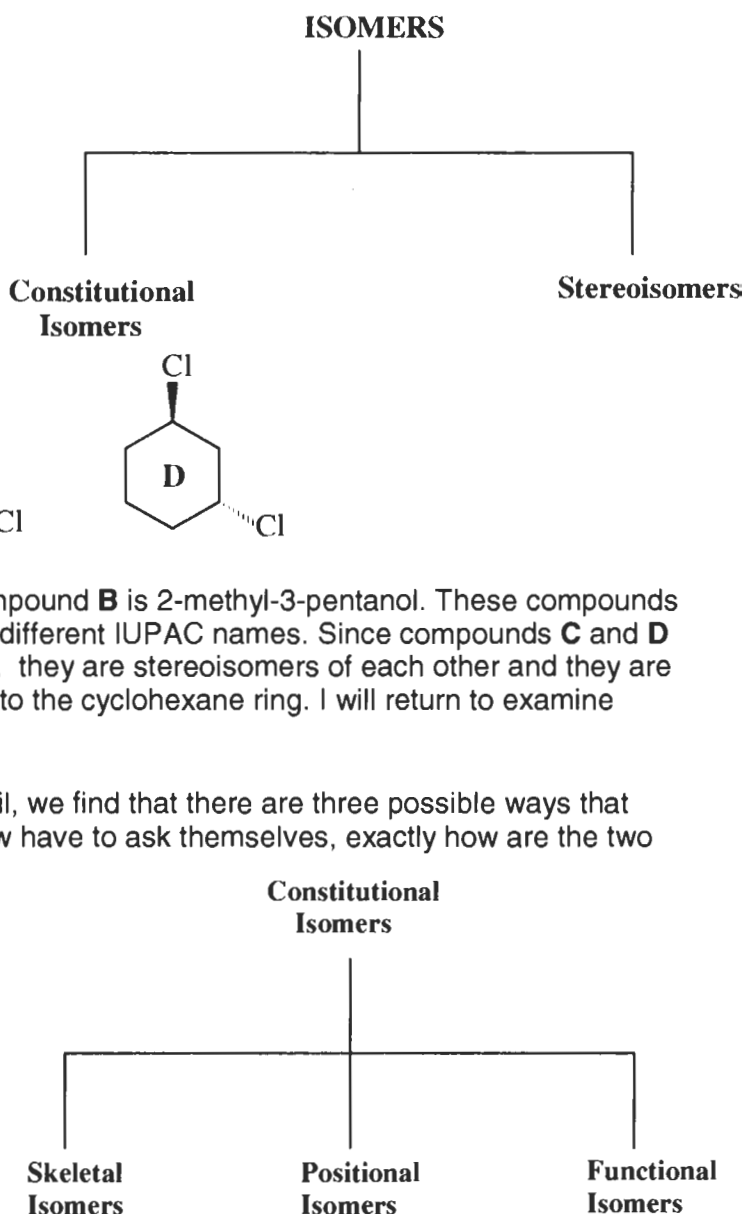


The name of compound **A** is 3-hexanol, the name of compound **B** is 2-methyl-3-pentanol. These compounds are constitutional isomers of each other since they have different IUPAC names. Since compounds **C** and **D** both have the same name; i.e., 1,3-dichlorocyclohexane, they are stereoisomers of each other and they are different in the way that the two Cl atoms are connected to the cyclohexane ring. I will return to examine stereoisomers in more detail later in **Part 3** of this series.

If we now consider constitutional isomers in greater detail, we find that there are three possible ways that isomers may have different names. The students will now have to ask themselves, exactly how are the two compounds different?

The second question is: Do the two constitutional isomers contain different functional groups?

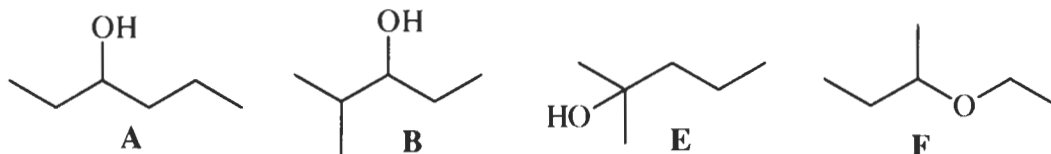
If the answer is **YES**, then the compounds are **functional isomers** of each other. If the answer is **NO**, then **we must ask another question**.



The third question is: Do the two constitutional isomers (which contain the same functional group), contain the same number of carbon atoms in the longest chain?

If the answer is **YES**, then the **two constitutional isomers are positional isomers of each other**. If the answer is **NO**, then the **two constitutional isomers are skeletal isomers of each other**.

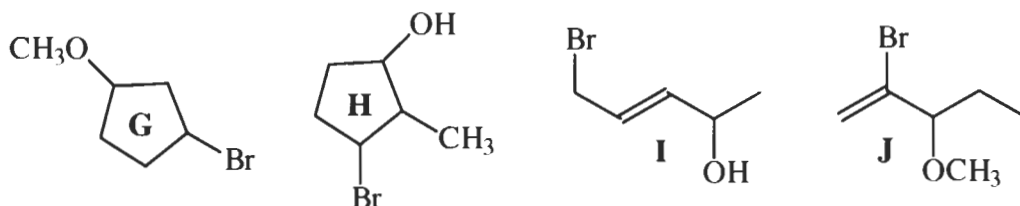
We can illustrate these terms by providing additional constitutional isomers to consider.



Compounds **A** (3-hexanol) and **B** (2-methyl-3-pentanol) are **skeletal isomers** as the longest chain containing the functional group is different. Compounds **B** and **E** (2-methyl-2-pentanol) are **positional isomers** as the position of the OH group has changed, but the length of the longest chain containing the functional group is the same. Compound **F** (2-ethoxybutane) is a **functional isomer** of the other three constitutional isomers **A**, **B** and **E**.

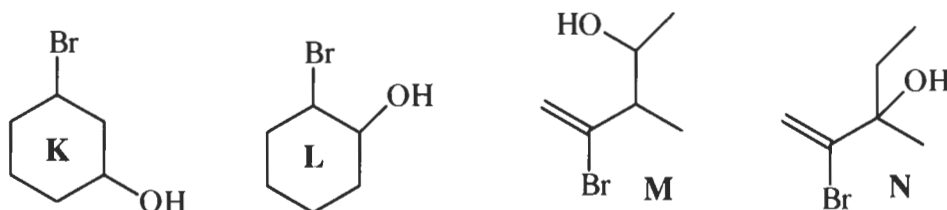
The students are now ready to move on to the concept of **degrees of unsaturation** and how it applies to the above discussion of isomeric structures. I have found that many of my students over my 37 times teaching the first semester of 2nd year organic chemistry have a great deal of difficulty understanding how a molecule that contains one degree of unsaturation does not necessarily have to be unsaturated. A saturated compound is one that has only sp^3 hybridized carbon atoms; an unsaturated compound is one that has at least one carbon atom that is not sp^3 hybridized. A saturated compound will therefore have only sigma bonds present, while an unsaturated compound will contain at least one pi bond.

Let us suppose that we wish to consider the possible structures possible for the formula $C_6H_{11}BrO$. The compounds will all contain one degree of unsaturation, but they could either be saturated or unsaturated. The following four compounds would represent two sets of functional isomers, both saturated and unsaturated.



Compound **G** (3-bromo-2-methoxycyclopentane) and compound **H** (3-bromo-2-methyl-1-cyclopentanol) are saturated functional isomers of each other. Compound **I** (6-bromo-3-pentene-2-ol) and compound **J** (2-bromo-3-methoxy-2-pentene) are unsaturated functional isomers of each other.

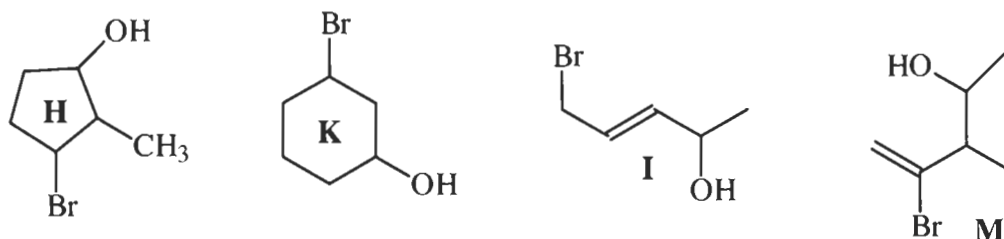
We can repeat the process for positional isomers.



Compound **K** (3-bromo-1-cyclohexanol) and compound **L** (2-bromo-1-cyclohexanol) are saturated positional isomers of each other. Compound **M** (4-bromo-3-methyl-4-pentene-2-ol) and compound **N** (4-bromo-3-methyl-4-

pentene-3-ol) are unsaturated positional isomers of each other.

We can repeat the process for skeletal isomers using some of the compounds from above.



Compound **H** and **K** are saturated skeletal isomers of each other, while compounds **I** and **M** are unsaturated skeletal isomers of each other. There are obviously many more possible compounds for the same formula C₆H₁₁BrO, I leave it to the readers to come up with additional structures to illustrate the various terms described above.

In **Part 3** of the series I will look at the various types of stereoisomers possible for a given formula.

AROMATIC DIRECTED LITHIATION CHEMISTRY: THEORY AND PRACTICE FOR ADVANCED UNDERGRADUATES PART 1.—INTRODUCTION

Dr. J. Norman Reed, Dept. of Chemistry
University College of the Cariboo

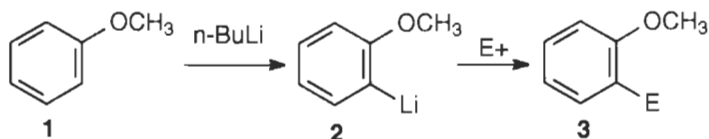
Anyone who teaches organic chemistry will be more than passingly familiar with the “classic” method of synthesizing multiply substituted benzene rings, namely, electrophilic aromatic substitution. In being familiar with this general reaction class, a chemist will also be acutely aware of the limitations of electrophilic aromatic substitution for the synthesis of, what at the outset, would seem rather simple multi-substituted (di, tri, tetra substituted etc.) aromatic rings. The limitations arise because the typical strongly activating groups that direct a second substitution (alkyl, -OH, -NHCOCH₃ for example), direct that substitution primarily to the para position and the common deactivating groups (notably -NO₂ and -C=O) direct the second substitution primarily to the meta position. As a result, there are numerous aromatic substitution patterns that are difficult to obtain by the classical electrophilic substitution route. This means that many simple aromatics, particularly those with contiguous substitution patterns, are difficult to synthesize, commercially expensive, and remain under exploited in synthetic organic chemistry. Numerous pharmaceutical target molecules include a large variety of aromatic structures and hence new and efficient methods of aromatic synthesis are under constant investigation in university and industrial labs. In 1939-1940 a new type of reaction was reported by



PHOTO 1: The amazingly intense and beautiful red-violet colour that is typical of an ortho-benzylic lithiated tertiarybenzamide. This solution is approximately 6 mmol of anion in 60 mL of THF. (Photo by Dr. Norman Reed, University College of the Cariboo)

Gilman and Bebb¹ and independently by Wittig and Fuhrman². They reported on the ortho deprotonation of anisole (**1**) (**Scheme 1**), and reaction of the resulting anion with various electrophiles (E⁺). The ether group acts as a "directing group" by coordinating to the lithium base and by acidifying the ortho proton. Coordination brings the base in to close proximity to the acidified proton. Today this chemistry is known as "directed ortho metalation" (DoM), and the directing groups are called "DMGs" (directed metalation groups)

SCHEME 1

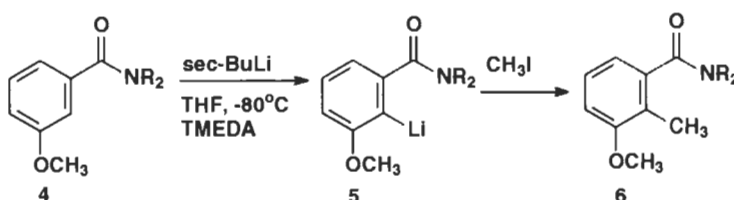


Additional studies on this reaction in terms of its reactivity and the scope of additional directing groups was reported in the 1960s and 70s. This time period was very comprehensively reviewed by Gschwend and Rodriguez³ in 1979. This review gave a number of researchers a much greater appreciation of the potential usefulness of DoM reactions.

In the rather auspicious year of 1979 this author had the good fortune to do his M.Sc. and, latter, his Ph.D. research, in the lab of Dr. Victor Snieckus⁴. Victor Snieckus is a Lithuanian born Canadian organic chemistry research scientist whose

contributions to DoM chemistry, starting in that year and continuing to the present day, have been nothing short of a high art form. Among a number of directing groups intensively investigated by the Snieckus research group and other research groups are tertiary benzamides⁵. In particular the diethyl and diisopropyl benzamides (**4**, R = Et or R = i-Pr) (**Scheme 2**) have proved to be very powerful directors of ortholithiation and are very useful in the synthesis of a wide variety of multi-substituted aromatic rings.

SCHEME 2

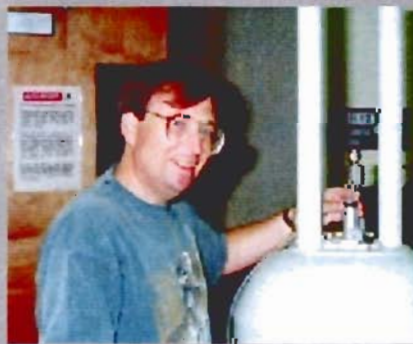


Scheme 2 illustrates a common feature of DoM chemistry, namely that when two directing groups have a meta relationship they work synergistically and direct lithiation between the groups, affording interesting contiguous substitution patterns (**6**). On their own, the tertiary benzamide groups are still excellent DMGs.

Another important feature of DoM chemistry is benzylic or "lateral" lithiation, as illustrated in **Scheme 3**. Here the even more acidic benzylic proton is easily and efficiently removed when it is ortho to a DMG, often giving very identifiable deep red to violet solutions, presumably because of the resonance of the anion with the aromatic ring. The photograph on **page 6**

Notes From the Editor

Norm Reed, University College of the Cariboo, Kamloops, BC



I must start this month's note with a sincere apology to all for the lateness of this issue. This issue was created with new software (new to me that is). The learning curve associated with the software, two research project students, and the constant flow of students through my office seeking help in one of my five different course/lab preps (yes, that's right, five (5)), have meant that I have often had to put the production of this issue aside. In future I plan to work the publication schedule back to March 1st, June 1st, September 1st and December 1st as mail-out dates. In order to keep things going I desperately need input from C3 members. Please, seriously consider submitting something! All the best to you in teaching and chemistry!N.R.

THE NEXT DEADLINE FOR SUBMISSION OF ARTICLES TO C3 NEWS IS MAY 20th, 2001—PLEASE CONTRIBUTE TO YOUR NEWSLETTER!

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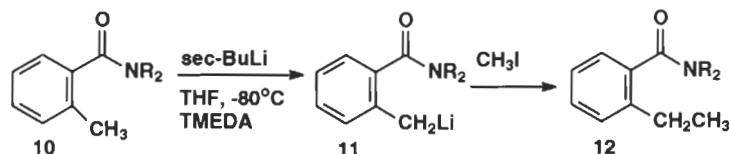
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(kindly generated by Marcus Hall, a very keen fourth year student, as part of his directed studies research project here at UCC) dramatically illustrates this colour feature of benzylic anions.

SCHEME 3



At present, DoM chemistry is of primary interest to research chemists and has not become a routine topic in undergraduate textbooks. As a powerful complement to traditional electrophilic aromatic chemistry I feel that it deserves more than passing mention in third or fourth year advanced organic courses. In addition, actual DoM reactions are pedagogically useful experiments for advanced undergraduate laboratories. I have endeavored to do just this over the past several years, that is, introduce advanced undergraduates to DoM chemistry both in lectures and the lab. In the lab DoM experiments are excellent vehicles for having students work experiments under inert atmosphere, at low temperature and using septum / syringe techniques for handling reagents. In addition, they typically make their own DMG containing starting materials, purify liquids by Kugelrohr distillation and isolate reaction products using flash chromatography as a separation method.

In future parts of this article I will summarize more about DoM chemistry and give detailed information on DoM experiments designed with undergraduates in mind.

References:

1. Gilman, H.; Bebb, R. L. *J. Am. Chem. Soc.* **1939**, *61*, 109.
2. Wittig, G.; Fuhrman, G. *Chem. Ber.* **1940**, *73*, 1197.
3. Gschwend, H. W.; Rodriguez, H. R. *Org. React. (N.Y.)* **1979**, *26*, 1.
4. Dr. Victor Snieckus, formerly professor of Chemistry at the University of Waterloo, and currently holder of the Alfred Bader Chair in Organic Chemistry at Queens University.
5. For an excellent and very comprehensive review of DoM chemistry and its application to the synthesis of novel polysubstituted aromatics see: Snieckus, V. *Chem. Rev.* **1990**, *90*, 879.