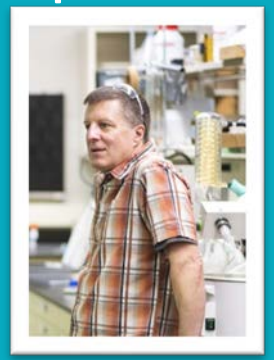
Seminar #5

July 3, 2020, 3:00 pm

Oligoynes, polyynes, and carbyne



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Carbon allotropes from sp^3-hybridized carbon (diamond) and sp^2-hybridized carbon (graphite, graphene, fullerenes, nanotubes) have well-established properties, many of which are technologically relevant. In particular, the discovery of fullerenes and graphene has captured the imagination of many chemists since these allotropes and their derivatives might serve as platforms for the next generation of electronic and energy capture devices. One needs to look no further than Nobel Prizes awarded in 1996 (C_{60}) and 2010 (graphene) to appreciate the impact of these discoveries. A carbon allotrope derived from sp-hybridized carbon atoms (carbyne) has been discussed since the 1960s,[1] although an authentic sample of "natural" carbyne has not yet been identified. Recent computational studies suggest that carbyne might be the strongest known material or the ideal molecular wire, although experimental confirmation of these predictions remains elusive and the search for carbyne continues.

Organic chemists have tackled the challenge of carbyne through the synthesis and study of model compounds. With this goal in mind, we have developed a new methods toward the synthesis of polyynes[2–3] and cumulenes[4] as compounds to model the properties of carbyne. These efforts provide us with a unique opportunity to explore the physical characteristics of these compounds as a function of length. This presentation will describe the evolution of properties in the progression of oligoynes, to polyynes, to carbyne. The contrast of various properties through correlations drawn from spectroscopic analyses and X-ray crystallography are key to these studies and will be discussed. Finally, some predictions for the properties of carbyne will be offered.

[1] A. El Goresy, G. Donnay, Science 1969, 161, 363–364
[2] W. A. Chalifoux, R. R. Tykwinski, Nat. Chem. 2010, 2, 967–971
[3] Y. Gao, Y. Hou, F. Gordillo-Gámez, M. J. Ferguson, J. Casado, R. R. Tykwinski, Nat. Chem. 2020, accepted
[4] J. A. Januszewski, R. R. Tykwinski, Chem. Soc. Rev. 2014, 43, 3184–3203

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