

Reaction of 1,3-diynes with Pentaphenylborole: A straightforward route towards phenyl-substituted Borirenes

Pedro H. R. Oliveira^{1,2}, Marieli O. Rodrigues^{1,2}, Caren D. G. da Silva^{1,2}, Merle Arrowsmith², Arumugam Jayaraman², Lukas Lubczyk², Cauê P. Souza³, Felipe Fantuzzi³, Eufiriano N. da Silva Júnior² and Holger Braunschweig¹

1) Institute for Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron, Julius-Maximilians-Universität Würzburg, 97074, Germany

2) Department of Chemistry, Federal University of Minas Gerais, UFMG, 31270-90, Brazil

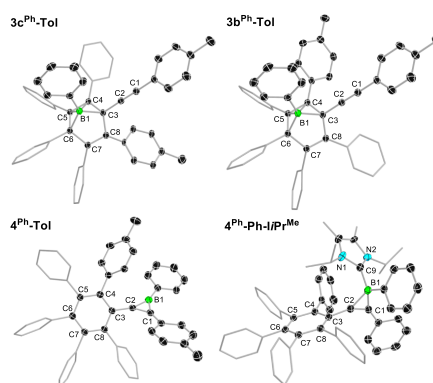
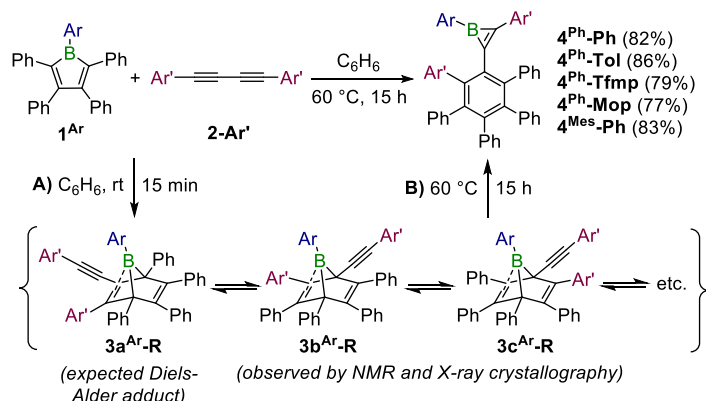
3) School of Chemistry and Forensic Science, University of Kent, Park Wood Rd, Canterbury CT2 7NH, United Kingdom

*e-mail eufirano@ufmg.br ; h.braunschweig@uni-wuerzburg.de

Keywords: Boron Chemistry, Boroles, Borirenes, Cycloaddition

ABSTRACT

Borirenes are isoelectronic to cyclopropenylum cation, thus representing the smallest type of boron-containing aromatic heterocycle.¹ Among different methods to synthesize borirenes the [2+1] cycloaddition of alkynes with *in-situ* generated borylenes has become a reliable strategy to access these compounds.² In recent years there has also been significant progress in the synthesis of boron-containing conjugated heterocycles by the ring expansion of borole precursors. The high reactivity of boroles, arises from their highly Lewis-acidic boron center and antiaromatic character, making them particularly prone to the insertion of multiple bonds generating more stable heterocycles.³ Considering previous studies between boroles and alkynes and the influence of the electronics and sterics of alkynes we describe a straightforward strategy for the synthesis of novel perarylated borirenes by combining pentaarylboroles with various 1,4-diarylbuta-1,3-diynes and explore the mechanism of these reactions both experimentally and computationally.



ACKNOWLEDGEMENTS

CAPES/DAAD/UFMG

REFERENCES

1. J. Wang, Q. Ye, *Chem. Eur. J.* **2023**, 202303695
2. H. Braunschweig, T. Herbst, D. Rais, S. Ghosh, T. Kupfer, K. Radacki, A. G. Crawford, R. M. Ward, T. B. Marder, I. Fernández, G. Frenking, *J. Am. Chem. Soc.* **2009**, *131*, 8989-8999
3. J. H. Barnard, S. Yruegas, K. Huang, C. D. Martin, *Chem. Comm.* **2016**, *52*, 9985-9991