PENN CENTER FOR INNOVATION
Empowering Ideas

Synthesis of Arylboronate Esters and Biaryl Compounds

Inventors
Virgil Percec
Brad Rosen
Christopher Wilson
Daniela Wilson

STATE OF DEVELOPMENT

Demonstrated in laboratory conditions with a wide array of substrates as well as various bases, catalysts, and ligands, showing range of applicability.

INTELLECTUAL PROPERTY

US#8,530,689

DESIRED PARTNERSHIPS

- License
- Co-development

REFERENCE MEDIA

Brad M. Rosen, Chenghong Huang, and Virgil Percec, "Sequential Ni-Catalyzed Borylation and Cross-Coupling of Aryl Halides via in Situ Prepared Neopentylglycolborane," Organic Letters; 2008; 10(12); 2597-2600.

Daniela A. Wilson, Christopher J. Wilson, Brad M. Rosen, and Virgil Percec "Two-Steps One-Pot Ni-Catalyzed Neopentylglycolborylation and Complementary Pd/Ni-Catalyzed Cross Couplings with Aryl Halides, Mesylates and Tosylates" Organic Letters, 2008 10(21) 4879-4882.

LEARN MORE

Pamela Beatrice
beatricp@upenn.edu
(215) 573-4513

Docket #U4807

Technology Overview

In particular aryl boronate esters and biaryls, are of interest for certain pharmaceutical and electronic material applications. Penn scientists have developed a chemical methodology for the sequential Ni-catalyzed borylation with a novel in-situ prepared reagent and Ni-catalyzed cross-coupling to form biaryls. This process is useful for the production of aryl boronate esters and biaryl compounds, key chemical building blocks and intermediates for the Sukuzi cross-coupling process.

Early results suggest that the process can be implemented as a three-step one-pot methodology comprising two-stages, one-pot in-situ preparation of neopentylglycolborane coupled with Ni-catalyzed borylation of aryl halides followed by complementary Ni/Pd-catalyzed cross-coupling with aryl bromides, iodides, chlorides mesylates, and tosylates. The latter two aryls are inexpensive coupling partners with arylboronic acids and provide a desirable method of carbon-carbon bond formation starting from phenols. This complementary approach gives rise to the rapid synthesis of biaryls, and demonstrates the synthetic competitiveness of in situ prepared neopentylglycolborane versus that of tetra(alkoxy)diboron derivatives.

Advantages

- The use of Ni-based catalyst, neopentylglycolborane, and simple dppe and dppp ligands, reduce the cost compared to diboron or Pd-based catalyst methods.
- Novel reagent, neopentylglycolborane, has potential or broad applicability, including metal-catalyzed borylation as well as uncatalyzed hydroboration.
- One pot method reduces time required and processing demands to reach the end product.

Applications

- Novel boronic acids and boronic esters for the synthesis of pharmaceuticals and other fine chemicals, in particular those with sensitive functionality.
- Processing of biaryls and potentially heterobiaryls for liquid crystalline systems, organic and polymer light emitting diodes (O/PLEDS) and other organic electronic materials.
- The stability of neopentylglycolborane in solution should allow for its production, storage, and likely purification and commercialization of the reagent.