I*t*Oct (I*t*Octyl) – pushing the limits of ItBu: highly hindered electron-rich N-aliphatic N-heterocyclic carbenes

Autorzy

Md. Mahbubur Rahman

Guangrong Meng

Elwira Bisz

Błażej Dziuk

Roger Lalancette

Roman Szostak

Michal Szostak

Rok wydania

2023

Czasopismo

Chemical Science

Numer woluminu

14

Strony

5141-5147

DOI

10.1039/d3sc01006f

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

I*t*Bu (**I*t*Bu** = 1,3-di-*tert*-butylimidazol-2-ylidene) represents the most important and most versatile *N*-alkyl N-heterocyclic carbene available in organic synthesis and catalysis. Herein, we report the synthesis, structural characterization and catalytic activity of **I*t*Oct** (I*t*Octyl), C_2-symmetric, higher homologues of **I*t*Bu**. The new ligand class, including saturated imidazolin-2-ylidene analogues has been commercialized in collaboration with MilliporeSigma: **I*t*Oct**, 929 298; **SI*t*Oct**, 929 492 to enable broad access of the academic and industrial researchers within the field of organic and inorganic synthesis. We demonstrate that replacement of the *t*-Bu side chain with *t*-Oct results in the highest steric volume of *N*-alkyl N-heterocyclic carbenes reported to date, while retaining the electronic properties inherent to N-aliphatic ligands, such as extremely strong σ-donation crucial to the reactivity of *N*-alkyl N-heterocyclic carbenes. An efficient large-scale synthesis of imidazolium **I*t*Oct** and imidazolinium **SI*t*Oct** carbene precursors is presented. Coordination chemistry to Au(I), Cu(I), Ag(I) and Pd(II) as well as beneficial effects on catalysis using Au(I), Cu(I), Ag(I) and Pd(II) complexes are described. Considering the tremendous importance of **I*t*Bu** in catalysis, synthesis and metal stabilization, we anticipate that the new class of **I*t*Oct** ligands will find wide application in pushing the boundaries of new and existing approaches in organic and inorganic synthesis.

Adres publiczny

http://dx.doi.org/10.1039/d3sc01006f

Strona internetowa wydawcy

https://www.rsc.org/