Mono-substituted amine-oligosilsesquioxanes as functional tools in Pd(II) coordination chemistry : synthesis and properties.

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Rok wydania

2020

Czasopismo

New Journal of Chemistry

Numer woluminu

44

Strony

10786-10795

DOI

10.1039/d0nj01568g

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Among the broad palette of POSS hybrids, the mono-functionalized ones can be considered as attractive starting blocks for further structural expansion. In this paper, we report on the poorly known group represented by N-containing derivatives which have great potential in many areas of organic and coordination chemistry. By using Buchwald–Hartwig amination, and starting from (3-aminopropyl)hepta(isobutyl)octasilsesquioxane and different aryl bromides, we obtained eight novel mono-substituted amine-POSS derivatives *via* C(sp^2)–N bond creation. In the next step, selected hybrids were used in metalation reactions by using palladium acetate. The driving force of this reaction is the formation of the metallacycle entity possessing the {Pd[N–H···O–C–O]} core, which is built by POSS attached amine fragments and acetate ligands, which points to a non-typical behavior in comparison to the conventional reaction between $Pd(OAc)_2$ and classical amines. The resulting coordination entities show very good solubility, which is not always possible with fully substituted POSS ligands and, which should be emphasized, is strongly demanded in potential applications, *e.g.* in catalysis. Herein, we report on the first palladium compounds containing mono-functionalized amine-POSS ligands, with a pseudochelate interaction stabilized by a hydrogen bond. For a detailed picture of the stability of the chelate rings maintained by hydrogen bonds, DFT calculations were carried out. Furthermore, the preliminary catalytic behavior of the resulting Pd(II) coordination compounds has been examined in the Suzuki–Miyaura coupling. All the obtained compounds were characterized by using EA, NMR (^{1}H, ^{13}C, ^{29}Si), and HR-MS.

Adres publiczny

http://dx.doi.org/10.1039/d0nj01568g