NEW FUNCTIONALIZED DERIVATIVES OF BIMESITYLENE AS PRECURSOR FOR OBTAINING OF POLYFUNCTIONAL LIGANDS

Vadim DRUȚĂ[1*], ORCID: 0000-0001-5527-6459
Vasile LOZAN[1], ORCID: 0000-0002-6951-6115

[1]*Institute of Chemistry, State University of Moldova, Chișinău, Moldova*

[*]Corresponding author: Vadim Druță, vaddr22@yahoo.com

An important class of organic compounds, which are found in many natural products, such as biologically active compounds, alkaloids or natural dyes, is represented by biaryls and their derivatives.

One of the interesting representatives of this family is bimesitylene due to the fact that, for steric reasons, the two conjugated aromatic rings are perpendicular to each other. In this molecule, the four aromatic hydrogen atoms are arranged at the corners of a tetrahedron, and their replacement by chelating functional groups could lead to derivatives capable of forming three-dimensional (3D) networks with metal ions. Thus, the synthesis of ligands based on functionalized derivatives of bimesitylene is promising for the subsequent assembly of metal-organic frameworks, as promising materials in sorption processes.

The aim of this study was the synthesis of the compound 3,3',5,5'-tetrakis(4-iodophenyl)-2,2',4,4',6,6'-hexamethyl-1,10-biphenyl, a precursor for obtaining new ligands, which was carried out in 4 successive stages.

At the initial stage, using 2-mesitylmagnesium bromide as a starting material, bimesitylene was synthesized with a yield of 60% through the Grignard reaction in an argon atmosphere and in the presence of the catalyst.

At the second stage of the synthesis, the product 3,3',5,5'-tetraiodo-bimesitylene was obtained by the interaction of bimesitylene with iodine in a strongly acidic medium [1].

The compound 3,3',5,5'-tetraiodobimesitylene was converted by Suzuki coupling reaction to 3,3',5,5'-tetraphenyl-2,2',4,4',6,6'-hexamethyl-1,10-biphenyl upon the interaction of 3,3',5,5'-tetraiodobimesityl with phenylboronic acid in the presence of Pd^0 catalyst by refluxing the reactant mixture under inert atmosphere. After the purification and recrystallization procedure from ethylacetate/hexane, the final product was isolated in 82% yield.

In the final step of the synthesis, tetraphenyl-bimesitylene was iodinated in the *para*-positions with iodine and the oxidizing agent bis(trifluoroacetoxy)iodobenzene (PIFA) for 24 h at room temperature. The desired compound 3,3',5,5'-tetrakis(4-iodophenyl)-2,2',4,4',6,6'-hexamethyl-1,10-biphenyl was obtained in ~70% yield after recrystallization from DCM/methanol.

The composition and structures of the synthesized compounds were confirmed by the physical methods of analysis - FTIR spectroscopy, GC MS, ^{1}H and ^{13}C NMR.

Keywords: bimesitylene, ligand, organic synthesis, physical methods of analysis.

References:

[1] Bahrin, L.G., Clima, L., Shova, S. *et al. Res Chem Intermed* **45**, 453–469 (2019).

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