Uniwersytet Wrocławski

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# N-Heterocyclic Carbene Complexes of Nickel(II) from Caffeine and Theophylline: Sustainable Alternative to Imidazol-2-ylidenes

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Streszczenie

Xanthines, such as caffeine and theophylline, are abundant natural products that are often present in foods. Leveraging renewable and benign resources for ligand design in organometallic chemistry and catalysis is one of the major missions of green and sustainable chemistry. In this Special Issue on *Sustainable Organometallic Chemistry*, we report the first nickel–*N*-heterocyclic carbene complexes derived from Xanthines. Well-defined air- and moisture-stable, half-sandwich, cyclopentadienyl [CpNi(NHC)I] nickel–NHC complexes are prepared from the natural products caffeine and theophylline. The model complex has been characterized by X-ray crystallography. The evaluation of steric, electron-donating, and π-accepting properties is presented. High activity in the model Suzuki–Miyaura cross-coupling is demonstrated. The data show that nickel–N-heterocyclic carbenes derived from both earth abundant 3d transition metal and renewable natural products represent a sustainable alternative to the classical imidazol-2-ylidenes.

Słowa kluczowe

Aromatic compounds, Cross coupling reaction, Hydrocarbons, Ligands, Pharmaceuticals

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