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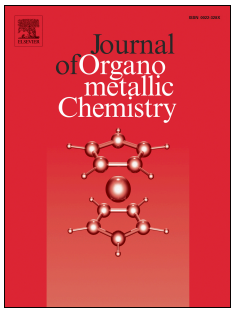

Mono and dinuclear bis(*ortho*-tolyl)platinum(II) compounds containing diethyl sulfide ligands: Synthesis, DFT studies and use as precursors in cycloplatination reactions

Ramón Bosque, Margarita Crespo, Anna Escolà, Mercè Font-Bardia

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ACCEPTED MANUSCRIPT

Mono and dinuclear bis(*ortho*-tolyl)platinum(II) compounds containing diethyl sulfide ligands: Synthesis, DFT studies and use as precursors in cycloplatination reactions

Ramón Bosque,[a,*] Margarita Crespo,[a,*] Anna Escolà,[a] Mercè Font-Bardia[b]

[a] *Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Facultat de Química, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.*

[b] *Unitat de Difracció de RX, Centres Científics i Tecnològics de la Universitat de Barcelona (CCiTUB), Universitat de Barcelona, Solé i Sabarís 1-3, E-08028-Barcelona, Spain*

Abstract

The synthesis of bis(*ortho*-tolyl)platinum(II) compounds containing diethyl sulfide ligands from $[PtCl_2(SEt_2)_2]$ and *ortho*-tolyl-lithium is presented. Formation of a dimer $[Pt(4\text{-}MeC_6H_4)_2(\mu\text{-}SEt_2)]_2$ is evidenced by ^1H NMR and HR-MS-ESI(+) spectra and the monomer *trans-anti*-$[Pt(2\text{-}MeC_6H_4)_2(SEt_2)_2]$ is characterized by X-ray diffraction analyses. Theoretical studies indicate that dimerization of the most stable form of the monomer (*cis-syn*) to the most stable conformer of the dinuclear species ($\alpha\beta\beta\alpha$) is favored (ΔE = -10.1 kJ/mol). The reactions of the dimer $[Pt(4\text{-}MeC_6H_4)_2(\mu\text{-}SEt_2)]$ with imine ligands $4\text{-}ClC_6H_4CH{=}NCH_2CH_2NMe_2$ and $2\text{-Br,6-}FC_6H_3CH{=}NCH_2Ph$ gave a tridentate [C, N, N'] five-membered and a bidentate [C, N] seven-membered platinacycles, respectively.

Keywords

Bis(*ortho*-tolyl)platinum(II) compounds, dimerization, DFT studies, cyclometalation, imine ligands.

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