

Synthesis of hexabenzocoronene based (NNC)Pt(II) acetylides

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Hexa-peri-hexabenzocoronenes (HBCs) provide a unique polyaromatic moiety for application in molecular electronic devices. HBCs with cyclometallated terdentate complexes of the type (NNC)M of Pt, Ru and Ir are having promising properties of harvesting light. New HBC based mono-and di-(NNC)Pt(II) acetylides (5) and (6) were prepared by CuI catalyzed coupling reaction and obtained orange solid products in 86% and 73% yield, respectively. The ligand (2) (LH) was prepared by Diels-Alder reaction between (1) and 2-cyanopyridine with 44% yield and the lactone by-product (3) was obtained in 16% yield. The ortho-metallated squareplanar platinum(II) complex [(L)PtCl] (4) was synthesized as a dark yellow solid in 83% yield from the reaction between(2) and $[PtCl_2(DMSO)_2]$ in boiling chloroform. All the new compounds were characterized by IR, Mass, ¹H NMR and ¹³C NMR spectroscopy. Further, the compounds (3) and (4) were confirmed by X-ray crystallography. The substitution of tertbutyl groups on the ligand and HBC successfully enhanced the solubility of HBC based (NNC)Pt(II) acetylides in organic solvents.



Keywords: Pt(II) acetylides, hexabenzocoronene, cyclometallation, lactone

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