Pd(II) Complexes of N- Allyl Substituted N- Heterocyclic Carbenes

F. Ekkehardt Hahn, Beate Heidrich, Thomas Lügger, and Tania Pape

Institut für Anorganische und Analytische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 36, D-48149 Münster, Germany

Reprint requests to Prof. Dr. F. E. Hahn. E-mail: fehahn@uni-muenster.de

Z. Naturforsch. 59b, 1519 – 1523 (2004); received August 31, 2004

Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

The unsymmetrically substituted imidazolium salt 1-ethyl-3-allyl-imidazolium bromide 1 was synthesized by treatment of imidazole with one equivalent each of n-butyl lithium and ethyl bromide followed by treatment with one equivalent of allyl bromide. The symmetrically substituted derivatives 1,3-diallyl-imidazolium bromide 2 and 1,3-bis(3-methyl-2-butenyl)-imidazolium bromide 3 were obtained from imidazole and two equivalents of allyl bromide or 4-bromo-2-methyl-2-butenyl bromide, respectively, in the presence of sodium hydrogencarbonate as a base. The imidazolium bromides 1–3 react with Pd(OAc)2 to afford the palladium(II) dicarbene complexes trans-[PdBr2(L)2] (L = 1-ethyl-3-allyl-imidazolin-2-ylidene, 4; L = 1,3-diallyl-imidazolin-2-ylidene, 5; L = 1,3-di(3-methyl-2-butenyl)imidazolin-2-ylidene, 6) by in situ deprotonation of the imidazolium salts. The X-ray structure analyses of 4–6 show all three complexes to be mononuclear with palladium(II) coordinated in a square-planar fashion by two carbene and two bromo ligands.

Key words: Carbene Ligand, Allyl Substituents, Palladium(II), Crystal Structure