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

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

The unsymmetrically substituted imidazolium salt 1-ethyl-3-allyl-imidazolium bromide $\mathbf{1}$ 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 $\mathbf{2}$ and 1,3-bis(3-methyl-2-butenyl)-imidazolium bromide $\mathbf{3}$ 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 $\mathbf{1}-\mathbf{3}$ react with Pd(OAc)₂ to afford the palladium(II) dicarbene complexes trans-[PdBr₂(L)₂] (L = 1-ethyl-3-allyl-imidazolin-2-ylidene, $\mathbf{4}$; L = 1,3-diallyl-imidazolin-2-ylidene, $\mathbf{5}$; L = 1,3-di(3-methyl-2-butenyl)imidazolin-2-ylidene, $\mathbf{6}$) by transtructure analyses of $\mathbf{4}-\mathbf{6}$ 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