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Novel palladacycle N-Heterocyclic carbene complexes with bidentate [C,N] and terdentate [C,N,N] and [C,N,O] Schiff bases. Synthesis, characterization and crystal structure analysis

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#### ACCEPTED MANUSCRIPT

# Novel Palladacycle N-Heterocyclic Carbene Complexes with Bidentate [C,N] and Terdentate [C,N,N] and [C,N,O] Schiff Bases. Synthesis, Characterization and Crystal Structure Analysis

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#### **Abstract**

Schiff base palladacycles readily reacted with *N*-heterocyclic carbenes (NHCs) after deprotonation of the corresponding imidazolium salts with K[N(SiMe<sub>3</sub>)<sub>2</sub>] to give mononuclear cyclometallated complexes in which the NHC was coordinated *trans* to the imine nitrogen. The reaction of dinuclear acetate-, **1**, or chloro-bridged, **2**, **3**, complexes gave new monoculear species, **4**–**9**, after the bridge–splitting reaction, inclusive of acetato/chloride exchange during the purification process. Treatment of the terdentate [*C,N,N*] metallacycles, **10**, **11**, with the NHCs gave **12**–**15** with substitution of the chloro or acetato ligands; the Pd–NMe<sub>2</sub> bond remains uncleaved. Reaction of the carbene ligands with the tetranuclear palladacycle, **16**, gave **17**–**20**, after splitting of the parent structure, but without ring opening of neither the Pd–N nor of the Pd–O bonds, hence retaining the metallated and coordination rings at the metal. The structures of **6**, **7** and **19** have been determined by single crystal X-ray diffraction.

Keywords: Palladacycles; Imidazolium salts; N-heterocyclic carbenes; Schiff base.

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