Non Classical *vs.* Classical Metal···H_3C-C Interactions: A Neutron Diffraction Study of a 14-Electron Ruthenium(II) System

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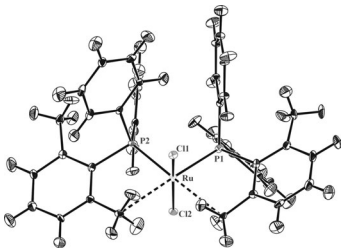
A neutron diffraction study establishes the precise nature of the δ agostic interactions in the complex $RuCl_2[PPh_2(2,6\text{-}Me_2C_6H_3)]_2$ (**1**). By contrast to the classical agostic bonding, it is shown that two ortho-methyl group of the xylyl substituents interact with the unsaturated metal centre through two C-H bonds each. The result is also substantiated by the NMR data in solution. [1], [2] Re-examination of all the X-ray structures with β, γ, δ and ε M···H_3C-C moieties as well as DFT calculations on models of **1** allow to conclude that the agostic interactions span the range between the classical (M···η^2-HC) and the non-classical (M···η^3-H_2C) types, depending on the number of atoms between the metal and the methyl group.



[1] Baratta W., Mealli C., Herdtweck E., Ienco A., Mason S. A., Rigo P., *J. Am. Chem. Soc.*, 2004, **126**, 5549. [2] Baratta W., Herdtweck E., Rigo P., *Angew. Chem. Int. Ed.*, 1999, **38**, 1629.

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