

The first copper complexes bearing the 1,3,5-triaza-7-phosphaadamantane (PTA) ligand.

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The Cu^I compound [Cu(PTAH)₄](NO₃)₅ (**1**) {PTAH = *N*-protonated form of 1,3,5-triaza-7-phosphaadamantane (PTA)} was easily prepared by reacting hydrated Cu(NO₃)₂ and PTA in aqueous acidic solution at room temperature. Further treatment of **1** with sodium hydroxide in water led to an unprotonated PTA derivative [Cu(PTA)₄](NO₃) (**2**). Both compounds are water-soluble and air-stable, and were characterized by IR, ¹H-, ¹³C{¹H}-, ³¹P{¹H}- and ⁶³Cu NMR spectroscopy, FAB-MS(+), elemental and single-crystal X-ray diffraction structural analyses. They exhibit a nearly regular tetrahedral coordination environment about each copper centre filled by the phosphorus atoms of the four PTAH/PTA moieties, which show distinct and unusual geometrical arrangements if viewed along the P–Cu bonds. The ³¹P{¹H}- and ⁶³Cu NMR spectra of **2** in D₂O solution show spin coupling between the ³¹P and ⁶³Cu nuclei at room temperature. These compounds represent the first examples of Cu complexes bearing PTA or any derived ligand with a cage-like PTA core and expand the restricted family of aqua-soluble copper phosphane complexes.

Adres publiczny

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