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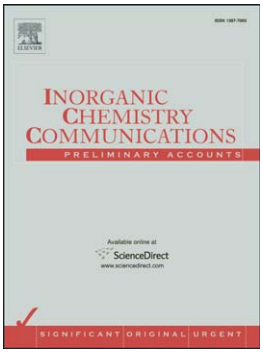

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ACCEPTED MANUSCRIPT

A cyclopalladated phosphine selenide with an anionic acylselenourea ligand

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Abstract

The chloro-bridged cyclometallated palladium(II) complex [PdCl{{κ*C*,*Se*-$C_6H_4P(Se)Ph_2$}]$_2$ reacts with 4-$MeC_6H_4C(O)NHC(Se)NEt_2$ in the presence of base to give [Pd{{κ*C*,*Se*-$C_6H_4P(Se)Ph_2$}{{κ*O*,*Se*-4-$MeC_6H_4C(O)NC(Se)NEt_2$}] in high yield. The complex was fully characterised by spectroscopic methods and also X-ray diffraction. This compound represents one of the few examples of a metal complex containing two different selenium-containing ligands.

Triphenylphosphine selenide (Ph_3P=Se) typically acts as a neutral, monodentate *Se*-donor ligand in complexes with transition metals including palladium, platinum and gold. A number of such compounds have been reported and several have also been structurally characterised. Examples include [$MX_2(Ph_3PSe)_2$] (M = Pt, Pd; X = Cl, Br, SCN), [$AuX(Ph_3PSe)$] (X = Cl, Br, I, CN) and also [$Au(Ph_3PSe)_2$]SbF_6 [1-9]. In several cases, cyclometallation can occur, forming compounds in which Ph_3PSe acts as a monoanionic *C*,*Se*-chelating ligand. To date cyclometallated triphenylphosphine selenide derivatives are known for Mn, Au, Pt and Pd [10-12]. It is worth noting, that while triarylphosphines can undergo cyclometallation reactions directly [13], triphenylphosphine selenide has to be converted into the Hg- Li- or Sn-derivatives to transmetallate the [{κ*C*,*Se*-$C_6H_4P(Se)Ph_2$]$^-$ group. We have previously investigated the chemistry and applications of heteroleptic metal complexes containing acylchalcogenourea ligands, which may either act as chelating *O*,*Se*$^-$ or monodentate *Se*$^-$ ligands [14-21]. Given that there are very few examples of metal complexes containing two different selenium donor centres, we thought the combination of a cyclometallated phosphine selenide with an acylselenourea might allow us to isolate such a compound. The reaction of the chloro-bridged palladium(II) dimer [PdCl{κ*C*,*Se*-$C_6H_4P(Se)Ph_2$}]$_2$ with 4-$MeC_6H_4C(O)NHC(Se)NEt_2$ in the presence of base afforded a yellow-orange compound (**1**) in high yield (Scheme 1) [22].

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