

# 2016

## INORGANICA

## PADOVA



### ATTI DEL CONGRESSO

**XLIV Congresso Nazionale  
di Chimica Inorganica**

Padova, 14 - 17 settembre



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA



Società Chimica Italiana

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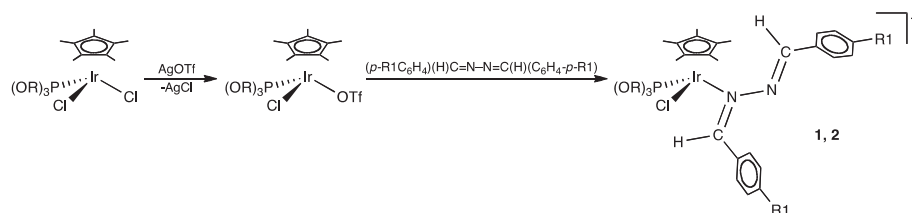
## Reactions of Azines with Half-sandwich Iridium Complexes. C–H Activation to Metalated Derivatives

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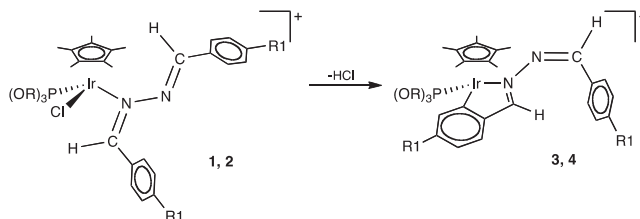
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Azine derivatives  $[\text{IrCl}(\eta^5\text{-C}_5\text{Me}_5)\{\kappa^1\text{-[N=C(H)(C}_6\text{H}_4\text{-}p\text{-R1)]N=C(H)-}$   
 $(\text{C}_6\text{H}_4\text{-}p\text{-R1})\}\{\text{P(OR)}_3\}]\text{BPh}_4$  (**1**, **2**) were prepared by reacting chloro compounds  
 $\text{IrCl}_2(\eta^5\text{-C}_5\text{Me}_5)[\text{P(OR)}_3]$  first with  $\text{AgOTf}$  and then with the appropriate azine.



$\text{P(OR)}_3 = \text{P(OMe)}_3$  (**1**),  $\text{P(OEt)}_3$  (**2**);  $\text{R1} = \text{H}, \text{CH}_3, \text{CH}_3\text{O}$ .

Complexes **1**, **2** undergo intramolecular C–H activation, affording metalated  
compounds  $[\text{Ir}(\eta^5\text{-C}_5\text{Me}_5)\{\kappa^2\text{-}(\text{C}_6\text{H}_3\text{-}p\text{-R1})(\text{H})\text{C}=\text{N}-\text{N}=\text{C}(\text{H})(\text{C}_6\text{H}_4\text{-}p\text{-R1})\}\{\text{P(OR)}_3\}]\text{-}$   
 $\text{BPh}_4$  (**3**, **4**).



Acetone azine  $(\text{CH}_3)_2\text{C}=\text{N}-\text{N}=\text{C}(\text{CH}_3)_2$  also gives the chelate complex  
 $[\text{Ir}(\eta^5\text{-C}_5\text{Me}_5)\{\kappa^2\text{-CH}_2(\text{CH}_3)\text{C}=\text{N}-\text{N}=\text{C}(\text{CH}_3)_2\}\{\text{P(OR)}_3\}]\text{BPh}_4$  (**5**) in the reaction  
with  $\text{IrCl}(\eta^5\text{-C}_5\text{Me}_5)(\kappa^1\text{-OTf})[\text{P(OR)}_3]$ .

The complexes were characterised spectroscopically (IR, NMR) and by X-ray  
crystal structure determination of  $[\text{Ir}(\eta^5\text{-C}_5\text{Me}_5)\{\kappa^2\text{-C}_6\text{H}_4(\text{H})\text{C}=\text{N}-\text{N}=\text{C}(\text{H})\text{C}_6\text{H}_5\}\text{-}$   
 $\{\text{P(OEt)}_3\}]\text{BPh}_4$ .