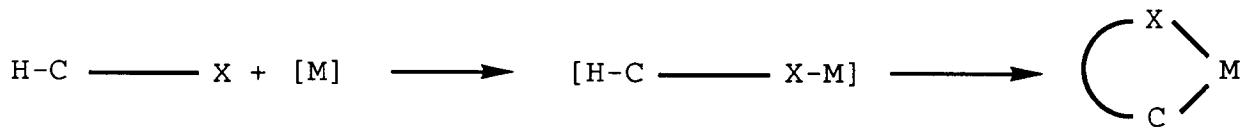


Interès de la reacció de ciclometal·lació:

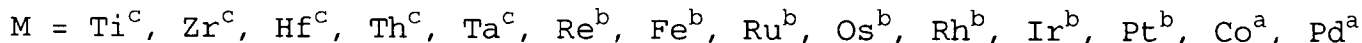
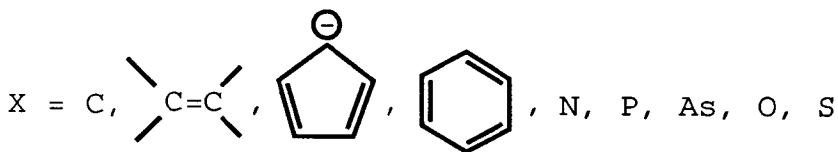
- aporta informació sobre el mecanisme d'activació C-H per compostos de metalls de transició
- és una reacció competitiva en l'activació intermolecular d'enllaços C-H
- aplicacions dels compostos ciclometal·lats:
 - * funcionalització selectiva de molècules orgàniques
 - * activitat antitumoral
 - * cristalls líquids

Mecanisme de la reacció de ciclometal·lació:



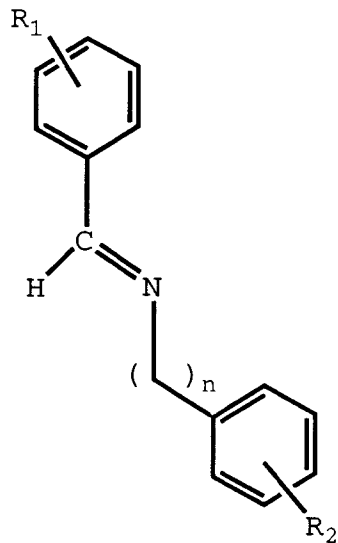
Mecanismes d'activació C-H:

- Substitució electròfila
- Addició oxidant
- Multicèntric



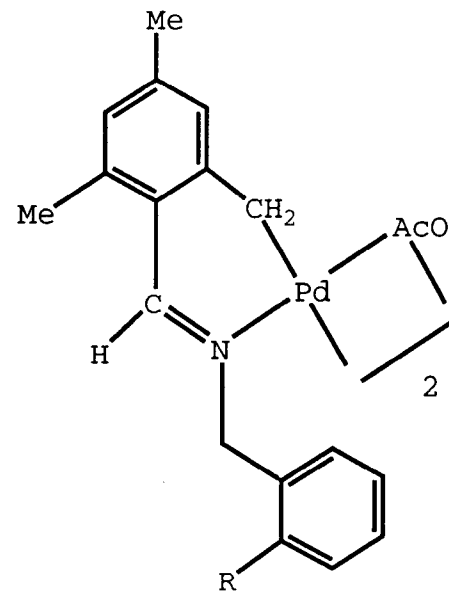
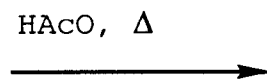
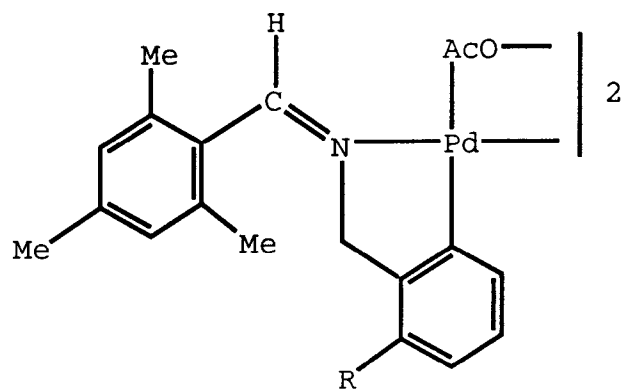
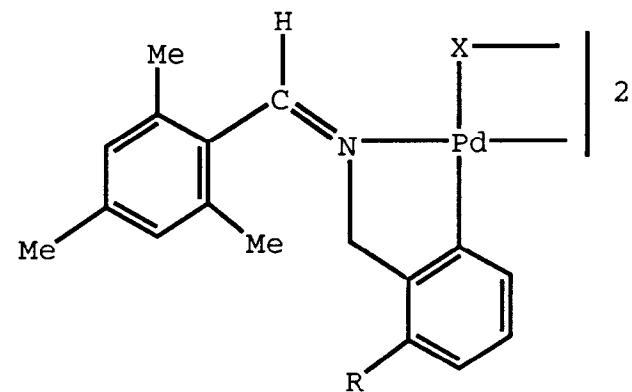
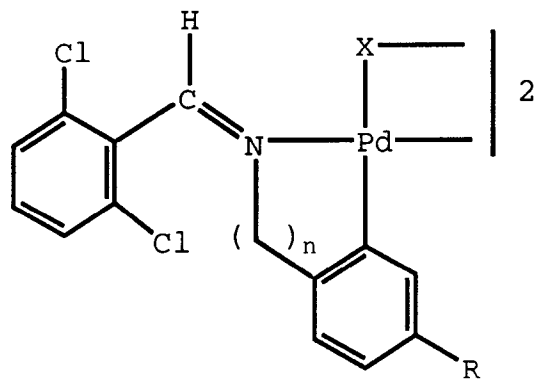
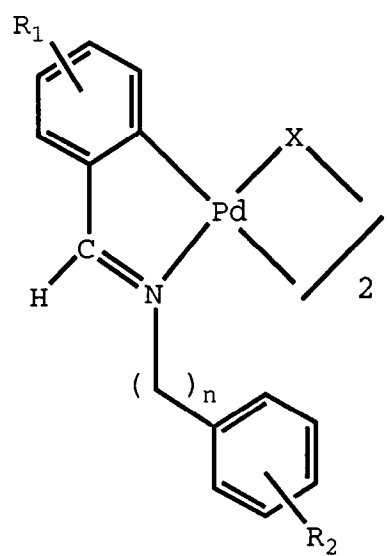
C = sp^2 (d'un anell aromàtic, d'un doble enllaç C=C, del ferrocè, d'un grup carbonílic o imínic) o sp^3 (d'un metil o el CH_2 d'un etil)

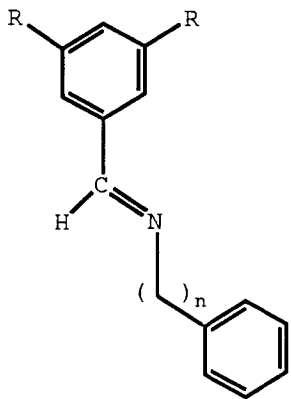
nombre de membres del metal·locicle = 3, 4, 5 o 6



Factors que poden influir en el procés de ciclopalladació:

- naturalesa electrònica i estèrica dels substituents
- inclusió o exclusió de l'enllaç C=N en el metal·locicle
- naturalesa sp^2 o sp^3 del carboni metal·lat
- nombre de membres del metal·locicle: 5 o 6

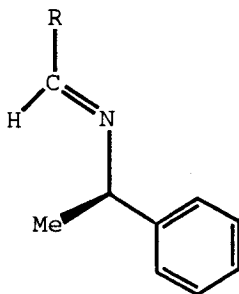




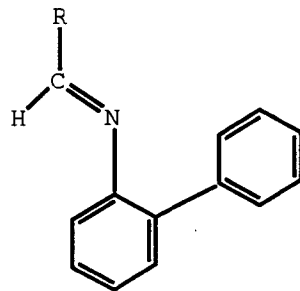
I

R = F o OMe

n = 0 o 1

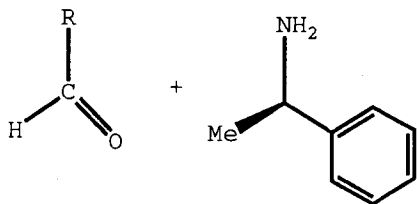


II

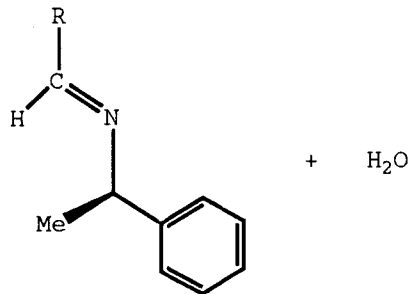


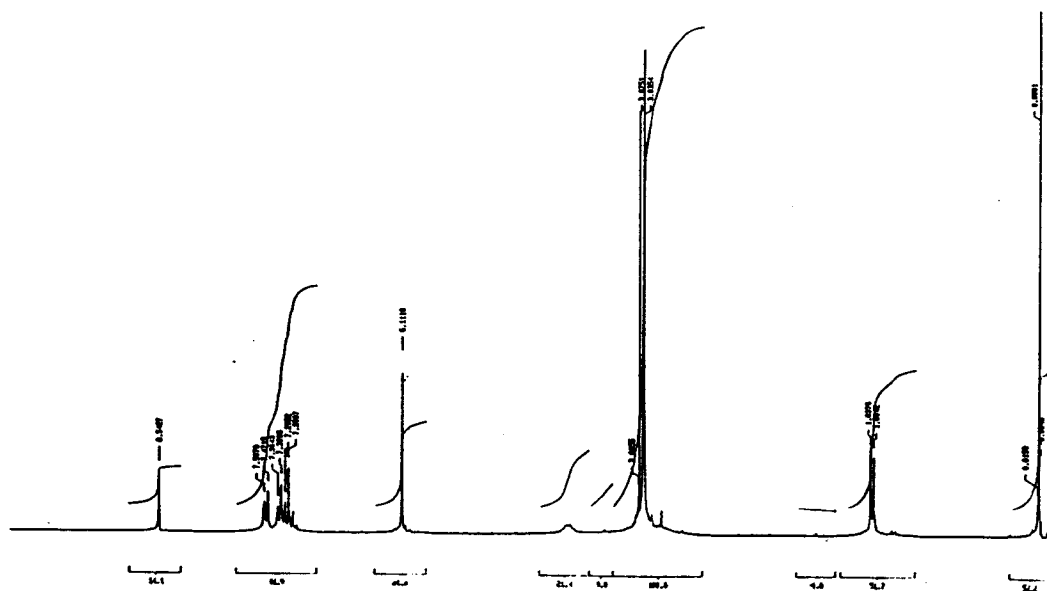
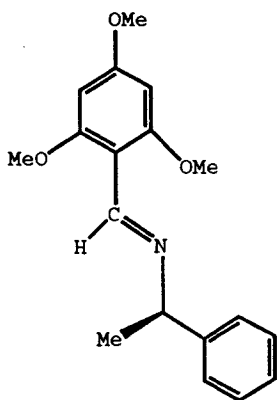
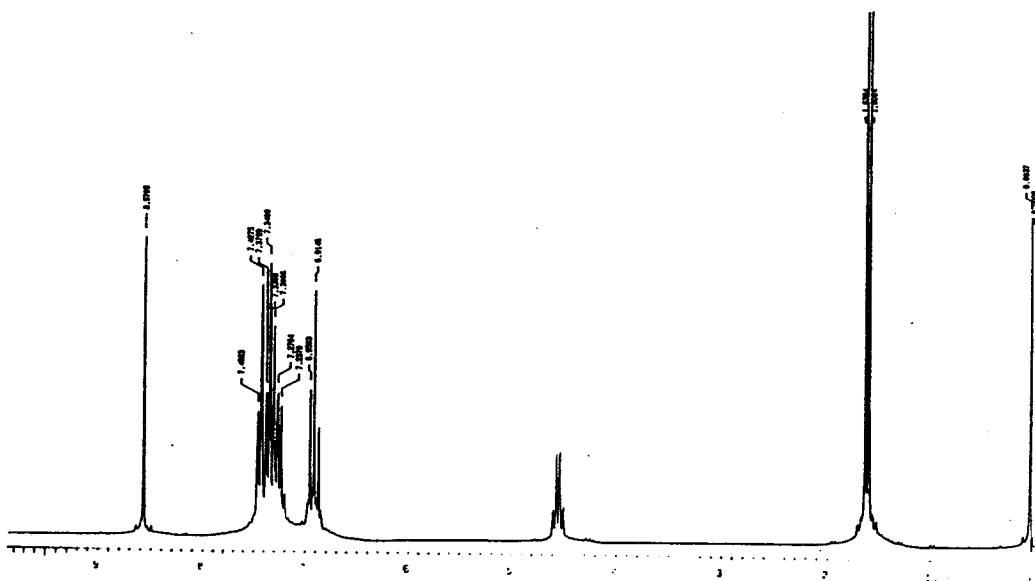
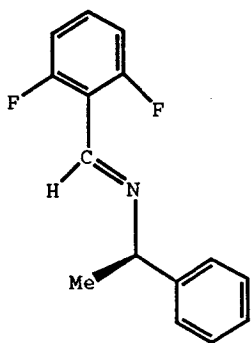
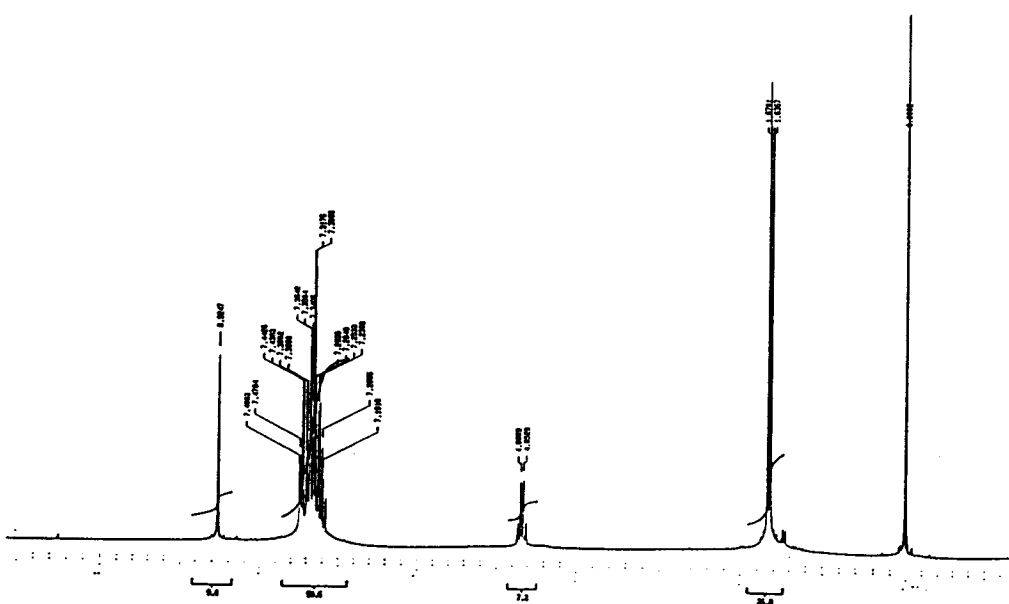
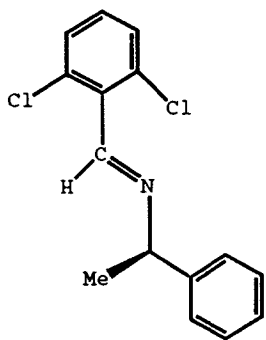
III

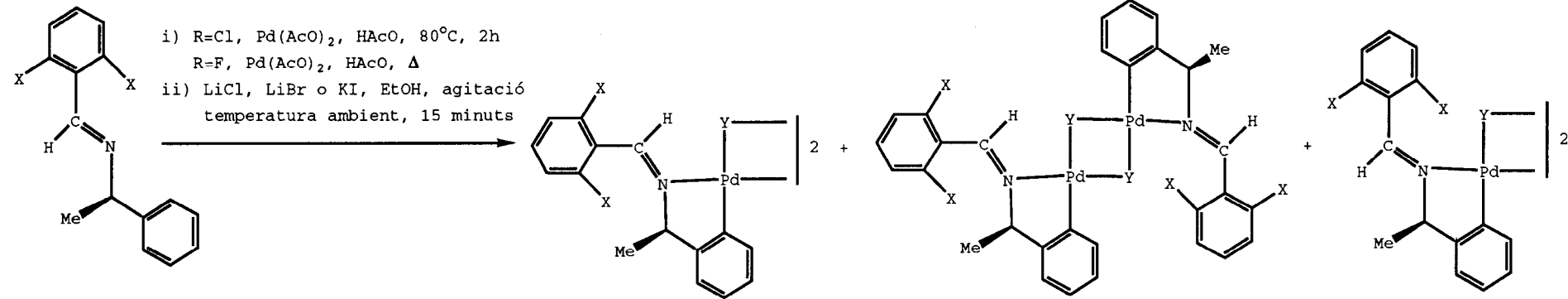
R = 2,6-Cl₂C₆H₃, 2,6-F₂C₆H₃ o 2,4,6-(MeO)₃C₆H₂

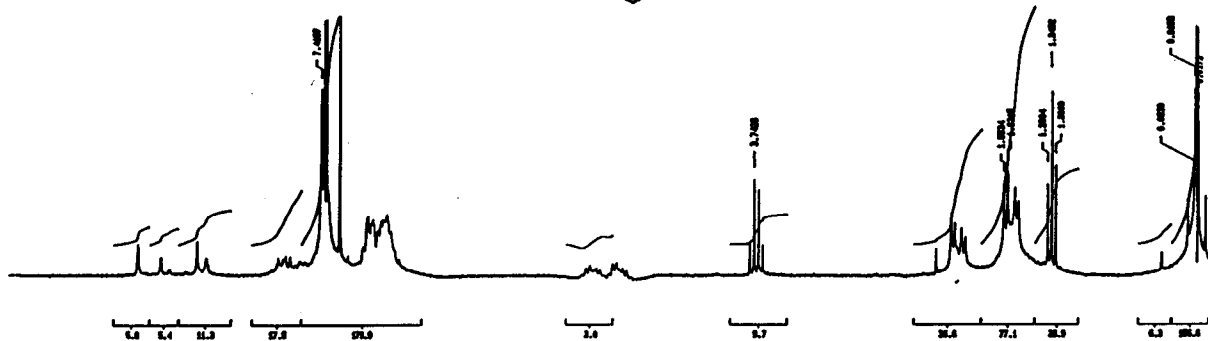
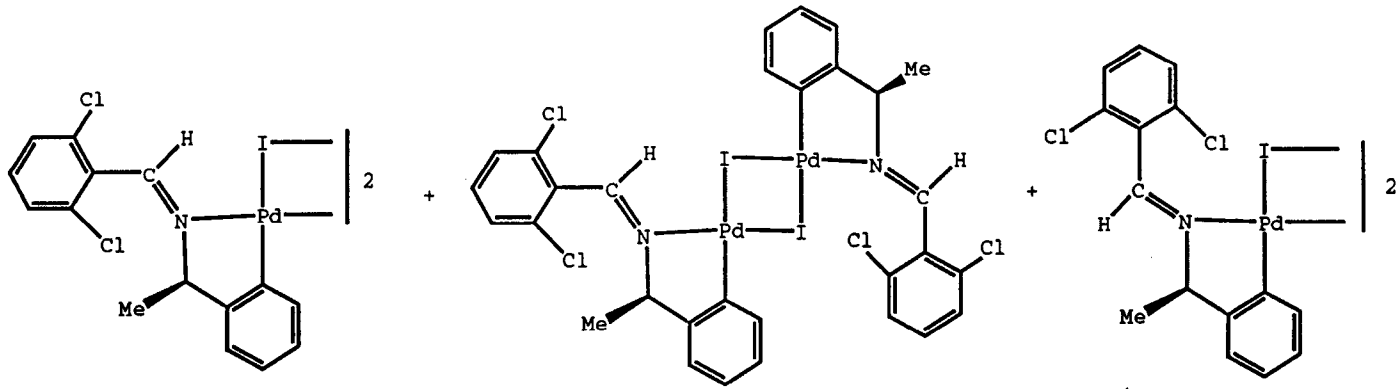


EtOH, Δ, 4 hores

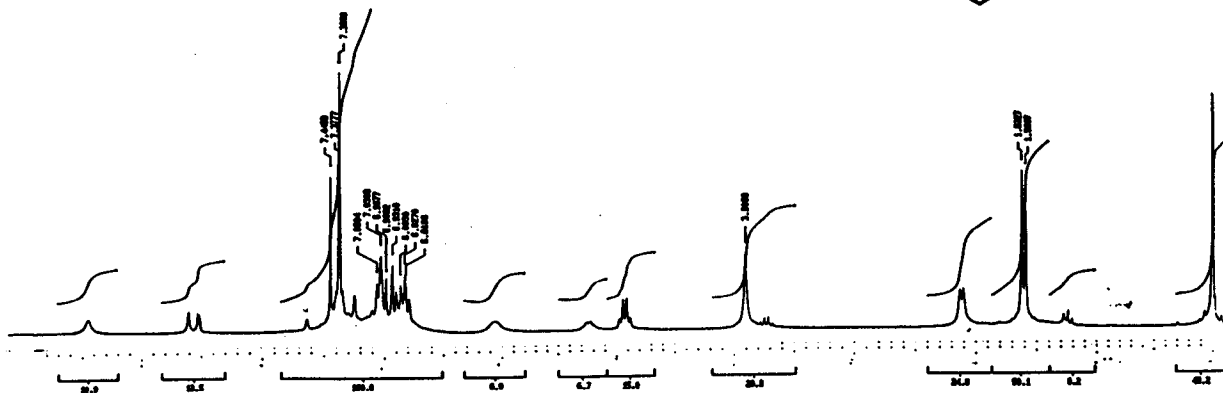
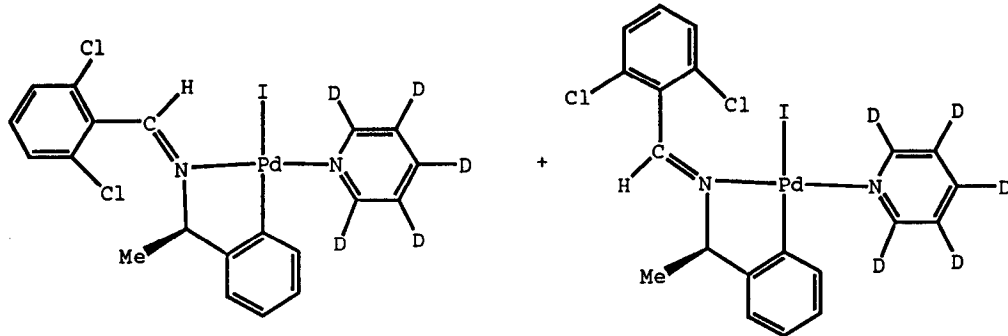








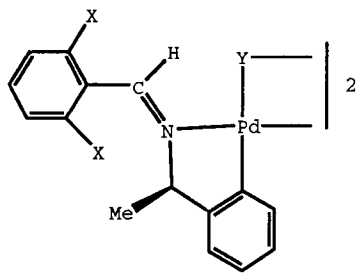
CDC13 + Py-d₅



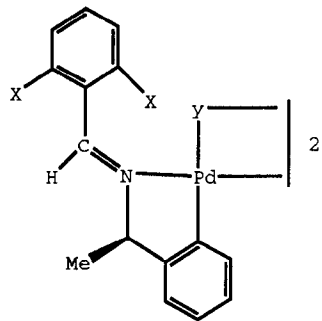
$\text{SiO}_2/\text{CHCl}_3$

Y = Cl o Br

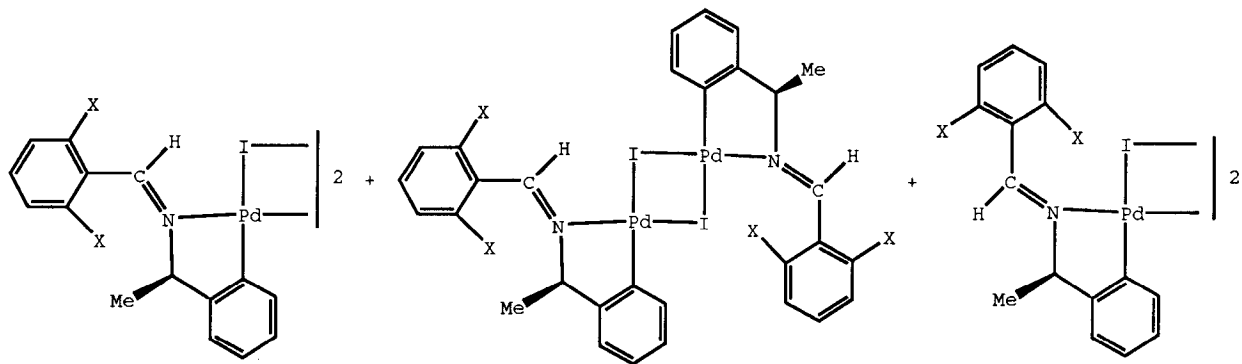
primera banda

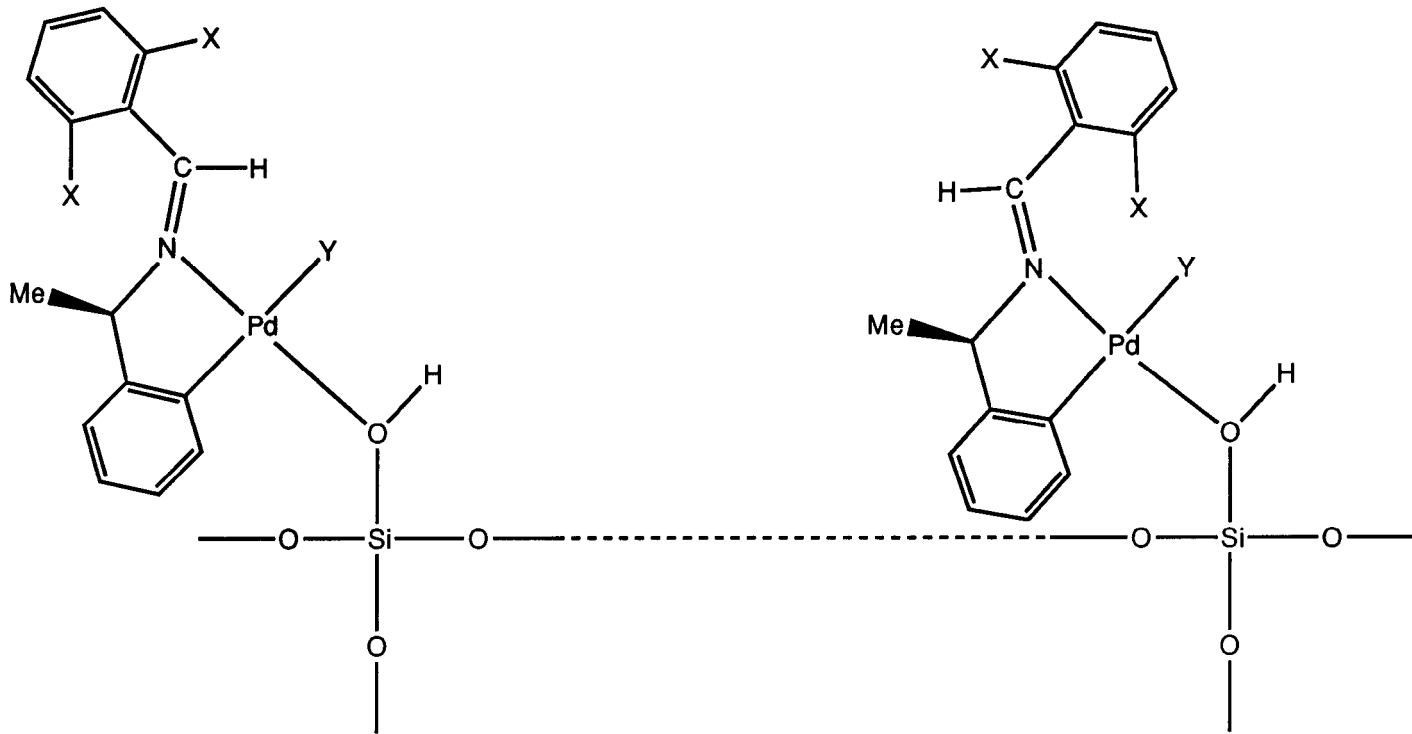


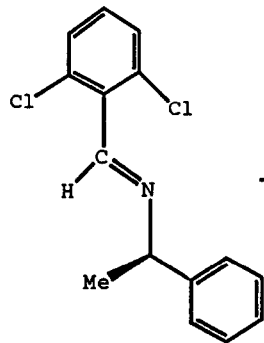
segona banda



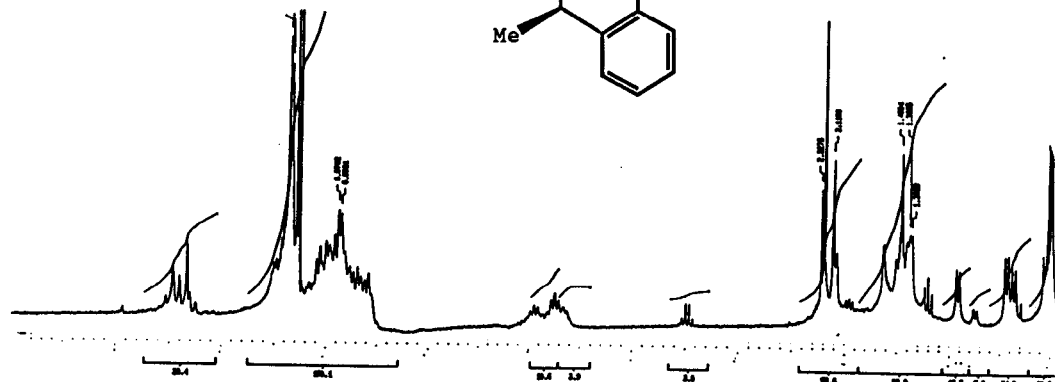
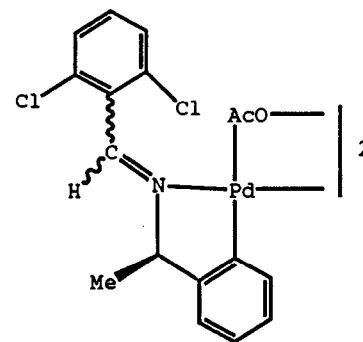
Y = I



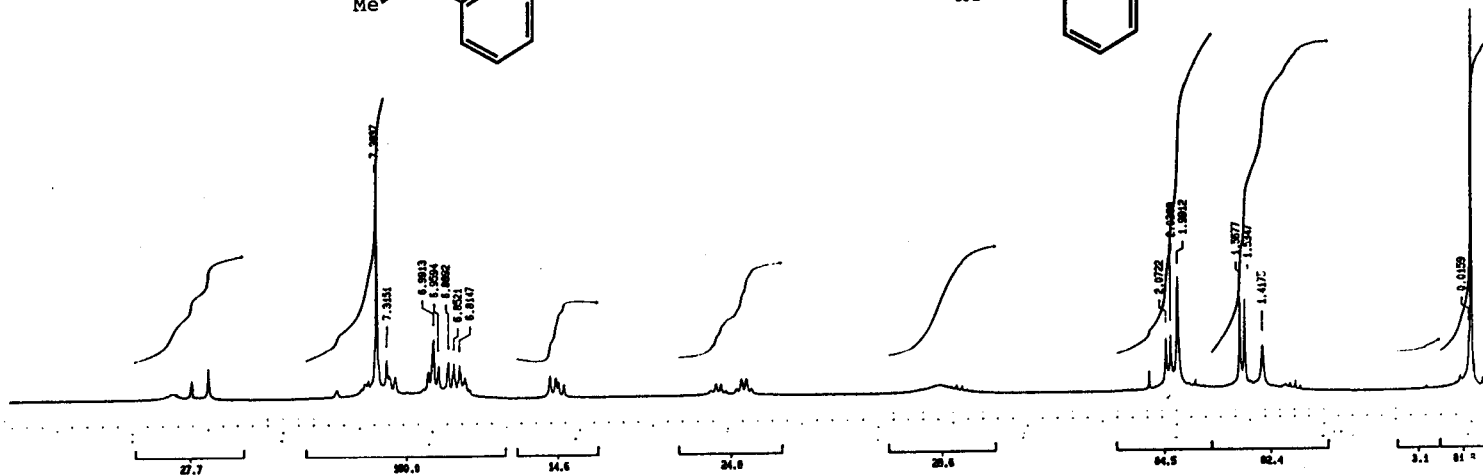
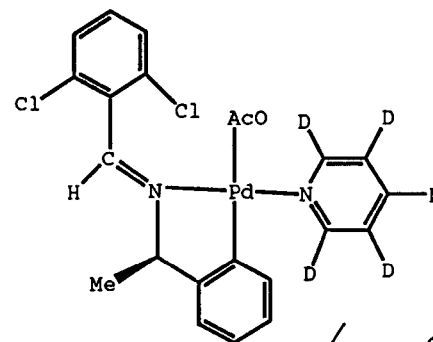
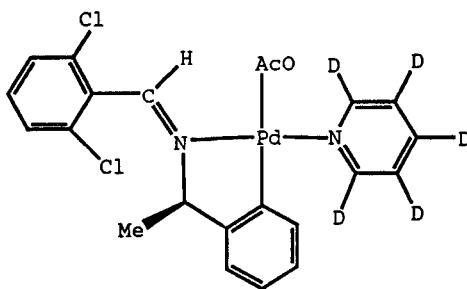


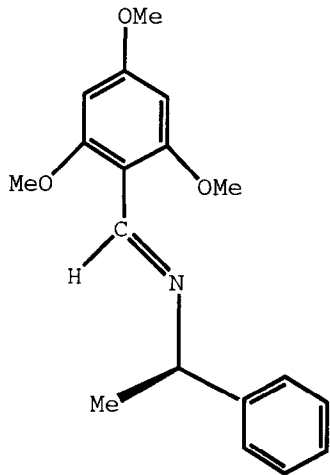


i) Pd(AcO)₂, HAcO, 80°C, 2h
 ii) SiO₂, CHCl₃/MeOH (100/2)

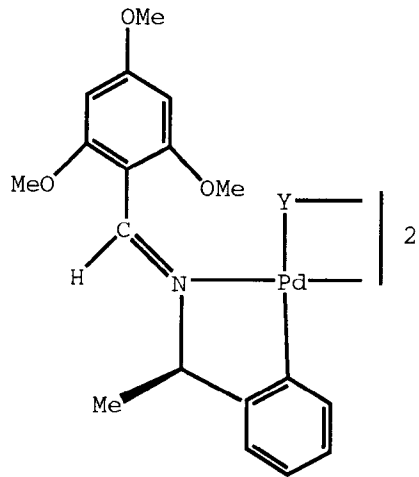


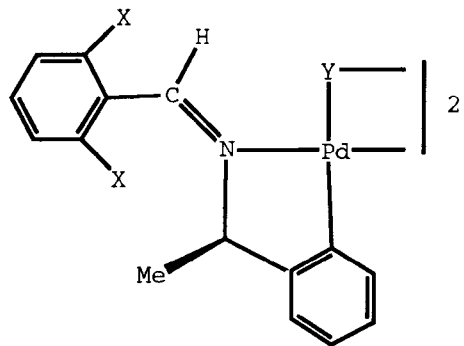
CDC13 + Py-d₅



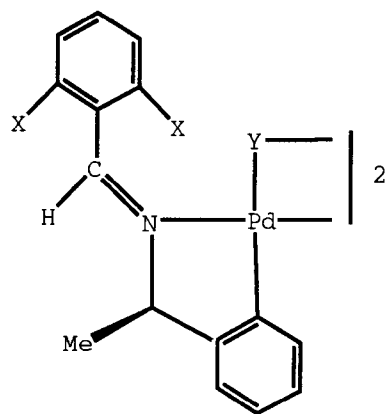
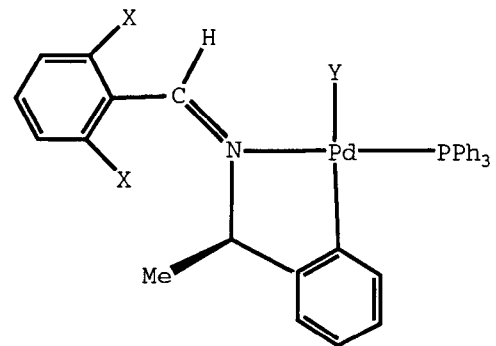


- i) $\text{Pd}(\text{AcO})_2$, HAcO , Δ
ii) LiCl , LiBr o KI , EtOH , agitació, temperatura ambient, 15 minuts
iii) $\text{SiO}_2/\text{CHCl}_3/\text{MeOH}$ (100/2)

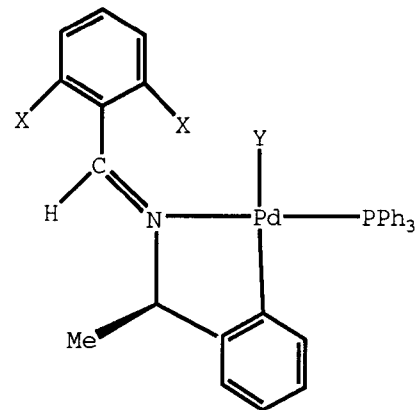


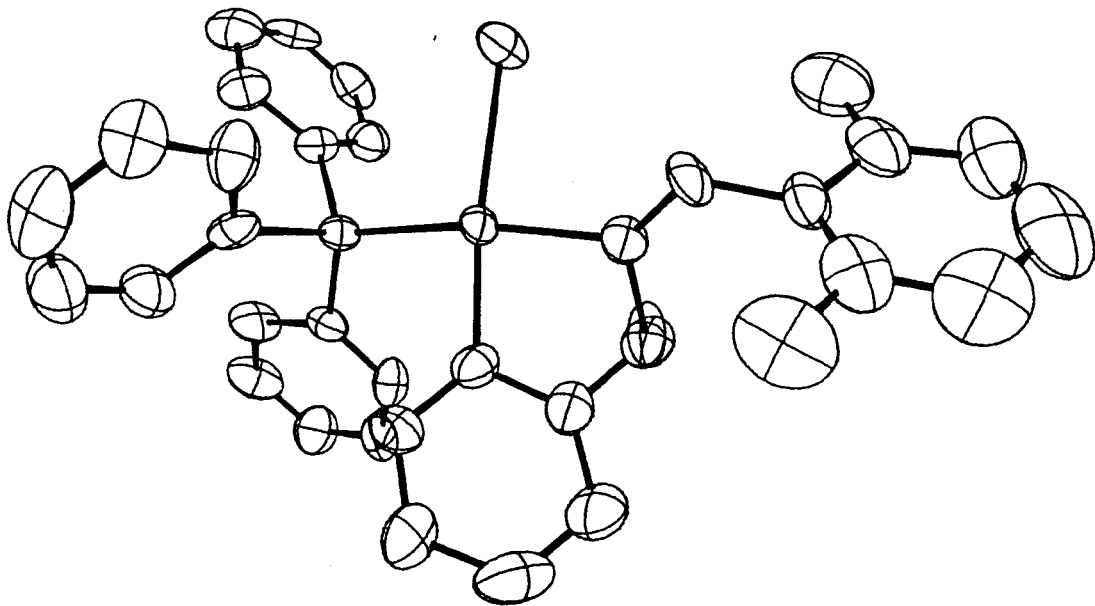
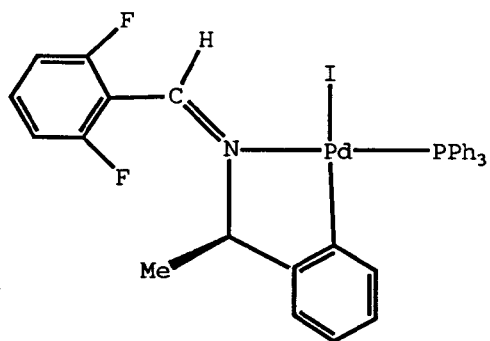


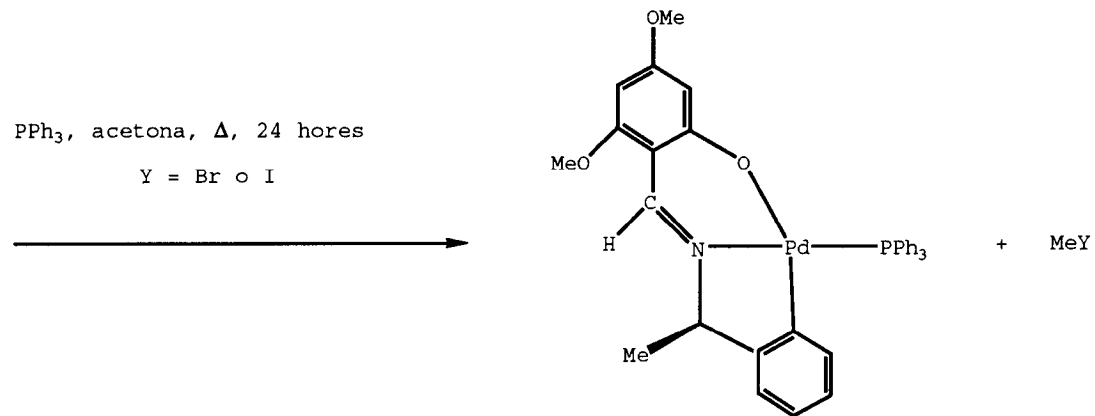
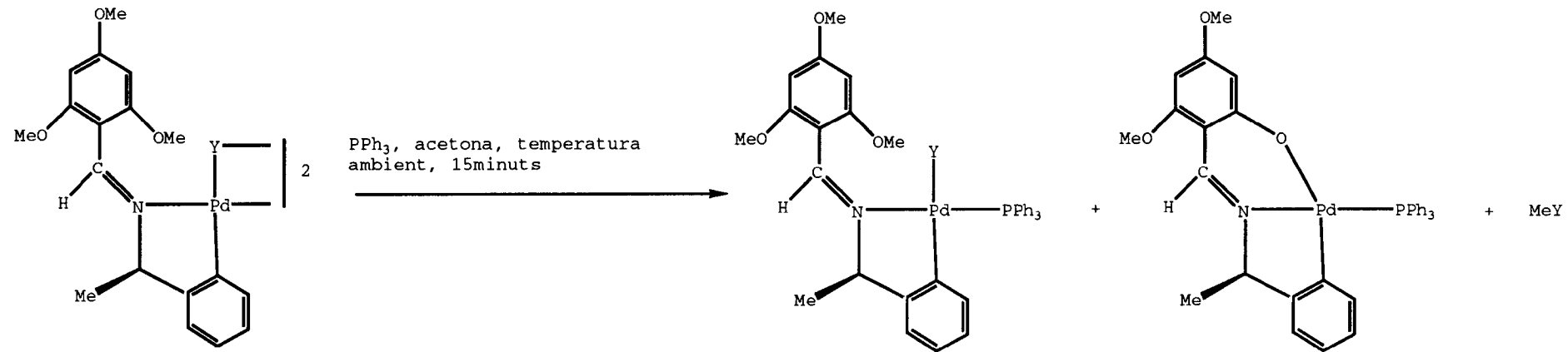
PPh₃, acetona, temperatura
ambient, 15 minuts

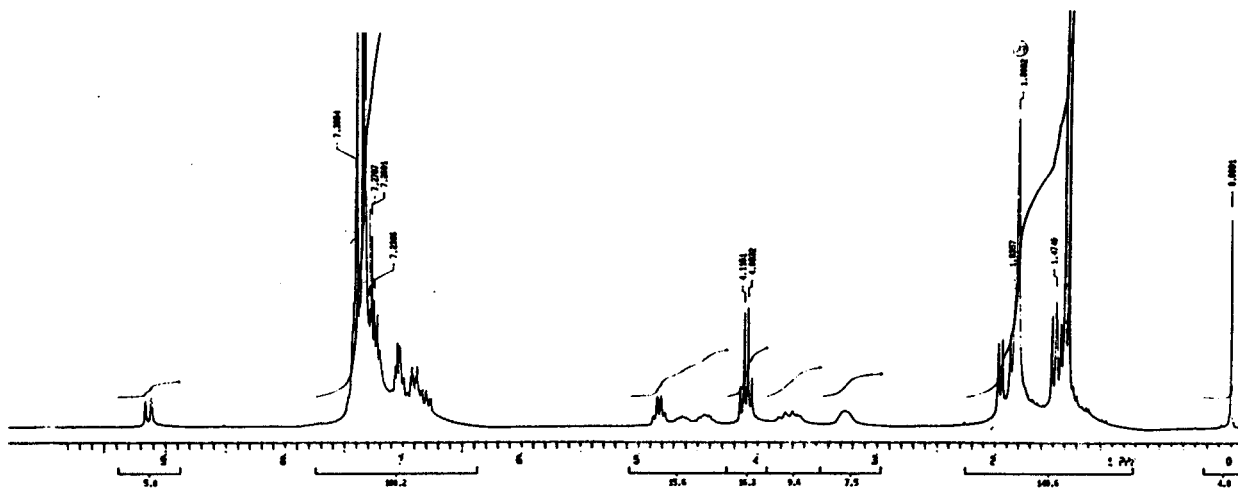
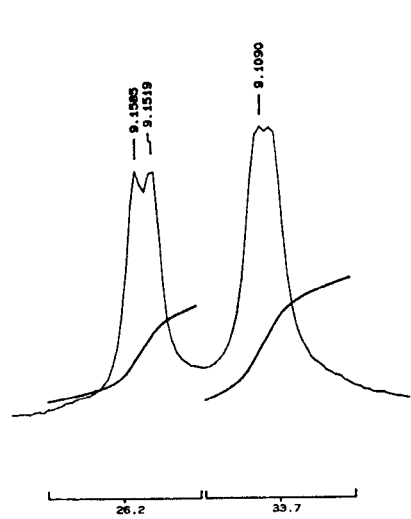
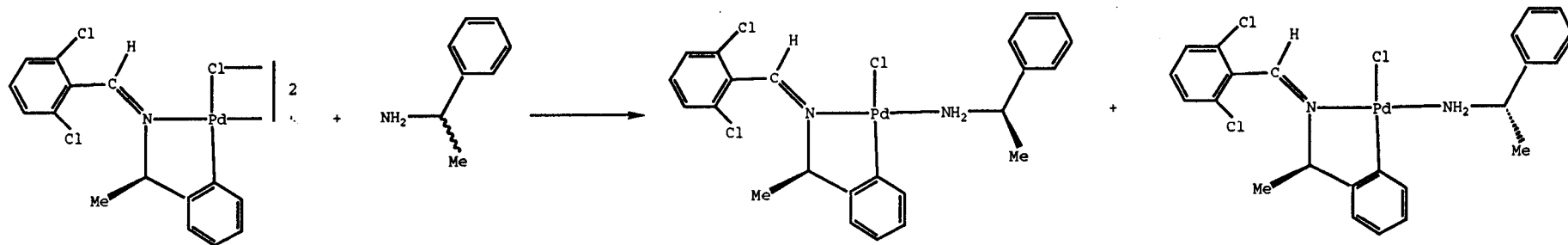
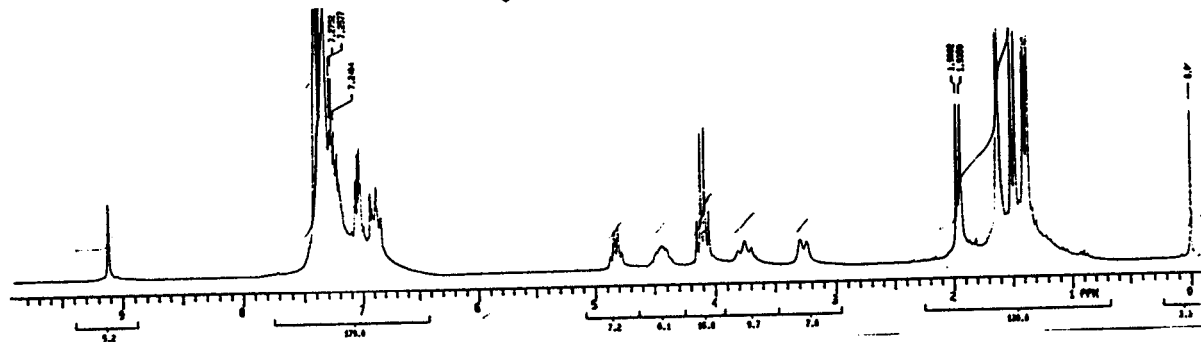
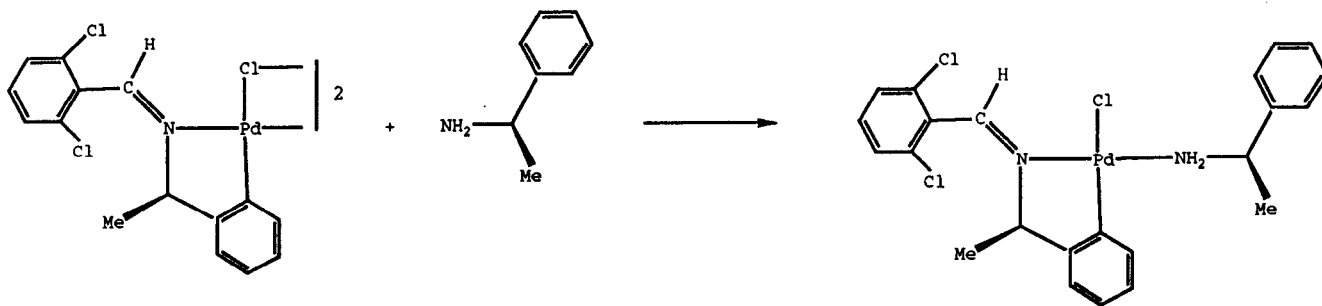


PPh₃, acetona, temperatura
ambient, 15 minuts









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