

# Activation of Carbon Chlorine Bonds with a bis(triphenylphosphine)dibenzylideneacetonepalladium Catalyst

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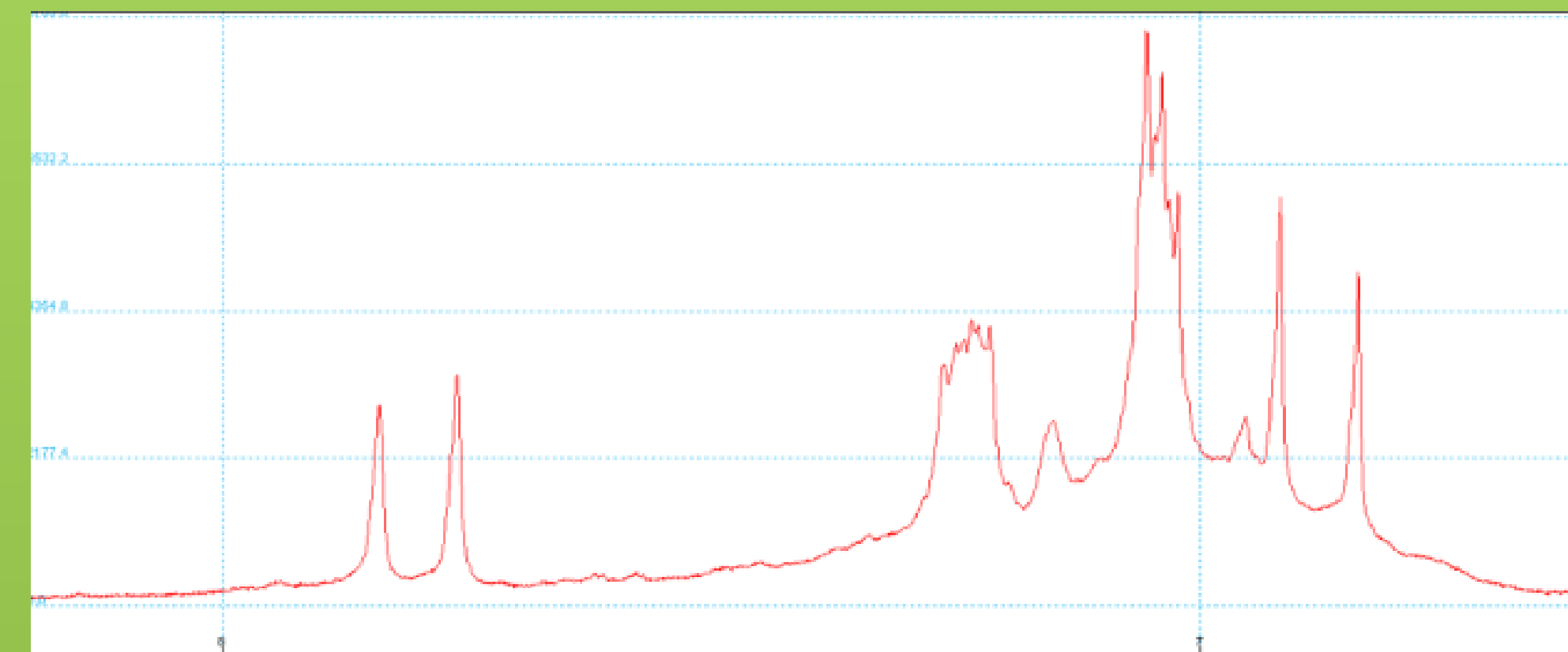
## Introduction

PCBs are commonly found in our environment for two main reasons. First, PCBs do not decompose easily, even though they can be destroyed by biological mechanisms. These mechanisms take a long time and if the concentrations are too high it will kill the bacteria. Second, PCBs are extremely lipophilic and have a very low vapor pressure. This means that the PCBs will not leach out into the air where it can be more exposed to photochemical degradation, but that it will sit in the soil and bioaccumulate in the fatty tissue of higher organisms. It is for these reasons that PCBs are listed as persistent organic pollutants, and need the intervention of people to have them removed from our environment. Buildings that contain dangerous levels of PCBs are abandoned and the land forsaken. There are commonly three methods for destroying PCBs. The first is directly overloading the C-Cl bonds with high energy levels introduced by incineration, irradiation, or plasma arc. Bacteria can break down PCBs by using them either as a carbon source, or by reductive dechlorination in which the chlorine is replaced with hydrogen. However, these are slow and highly selective processes. PCBs can be destroyed chemically using nucleophilic aromatic substitution but this process is relatively selective. Another method used is to expose the PCBs to high temperatures (~800°C) in the presence of hydrogen. This will cause the hydrogen to displace the chlorine and sever the C-C bond of the biphenyl. This process is not commonly used due to its extreme energy cost.

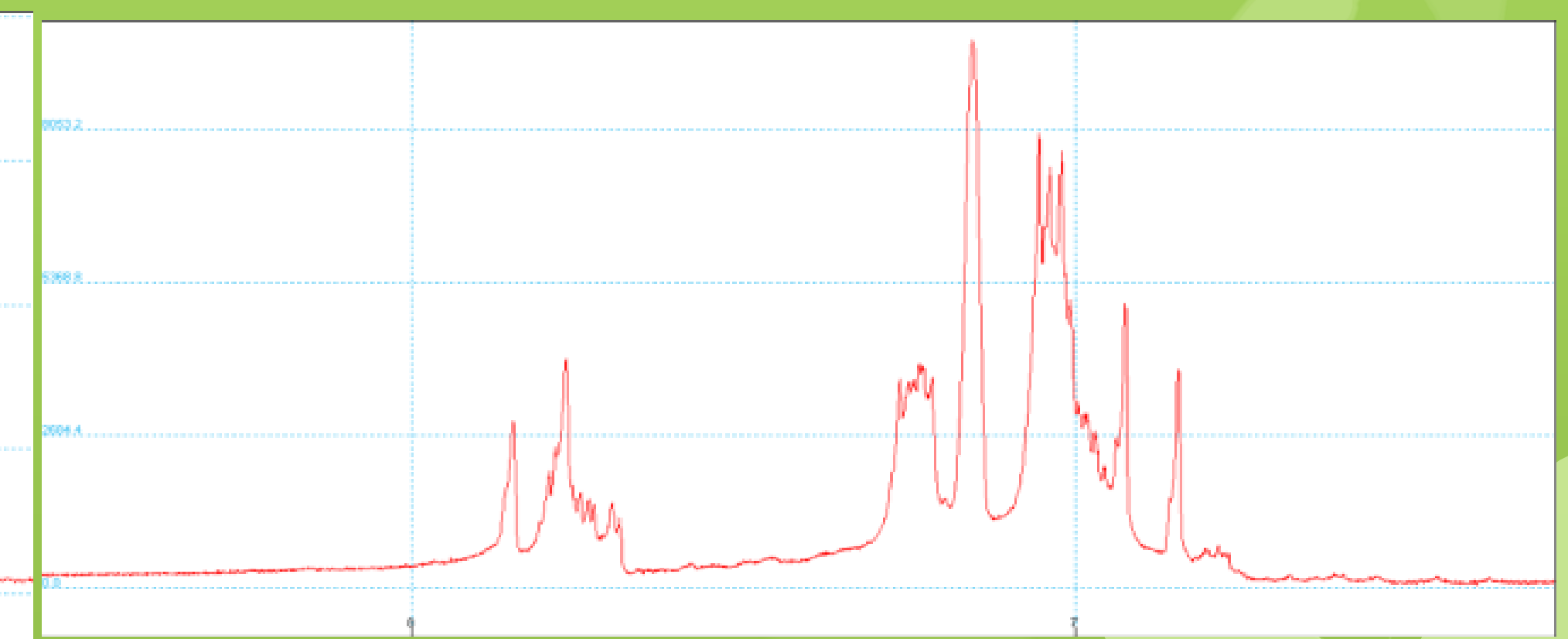
## Abstract

With the use of bis(triphenylphosphine)dibenzylideneacetonepalladium it is possible to activate carbon-chlorine bonds in chlorobenzene. The reaction forms a palladium-based complex that is far more reactive than the original carbon-chlorine bond. All reactants and products were characterized by <sup>1</sup>H NMR spectroscopy. The migration of a phenyl peak from 7.39ppm to 7.15ppm indicates the formation of a new complex that was determined to be chlorophenylbis(triphenylphosphine)palladium. The catalyst was also tested for reactivity with p-dichlorobenzene. The results of the p-dichlorobenzene analysis, though promising, were inconclusive. The crystals produced must be purified and further analyzed to confirm the dual bond activation.

Pre-Reaction Catalyst



Reaction Product

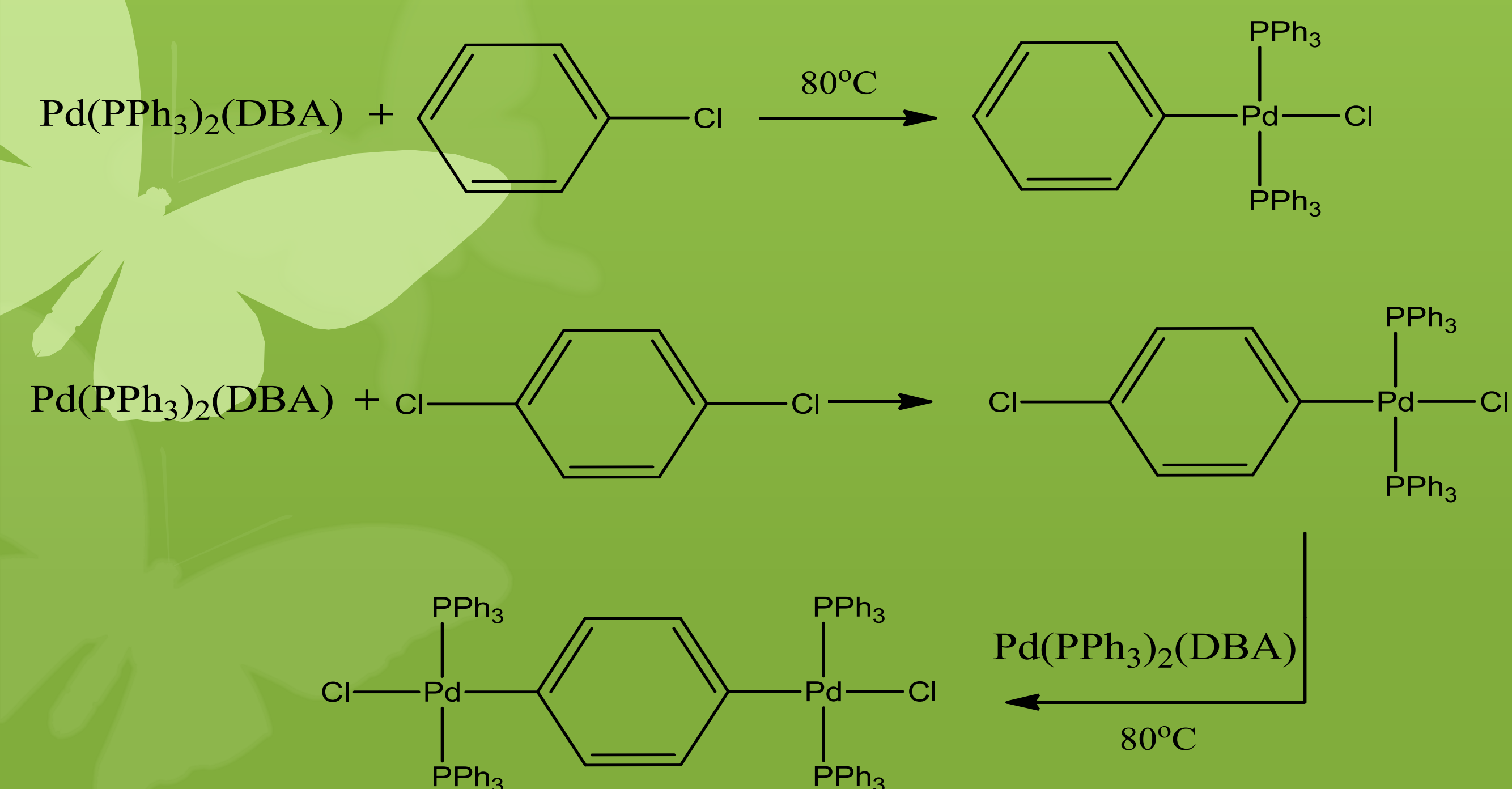


## Results and Discussion

Both spectra show the expected DBA doublets at 7.79ppm and 6.9ppm with the corresponding j values, as well as the peaks at 7.04ppm and 7.24ppm. When comparing the spectra of the unreacted tris(dibenzylideneacetone)palladium with the reaction product two characteristics stand out. First, the peak at 7.04ppm in the unreacted catalyst is leaning heavily to the right. In the reaction product the peak does not show any heavy leaning because it has acquired some triphenylphosphine character which would cause it to lean towards the left. The second peak to stand out is the large aromatic peak at 7.15ppm. It should also be noted that the expected triphenylphosphine peak at 7.39ppm was not found. This indicates that the phenyl peak has shifted, and possibly is overlapping with another new peak that is aromatic in nature. The shifted phenyl peak indicates the formation of a new complex that is most likely chlorophenylbis(triphenylphosphine)palladium.

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