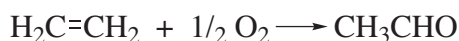


## Wacker Process

K. Sarath D. Perera

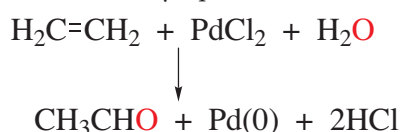
Senior Professor in Chemistry, Department of Chemistry, The Open University of Sri Lanka

Industrially, Wacker process is used to synthesise **acetaldehyde** by oxidizing **ethene** in the presence of  $O_2$  in the aqueous medium.  $PdCl_2$  and  $CuCl_2$  act as catalysts. The overall reaction is as follows.

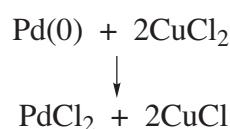


It is based on a combination of **three reactions**. They are:

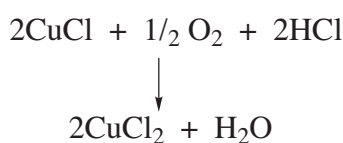
1. oxidation of ethene by aqueous Pd(II).



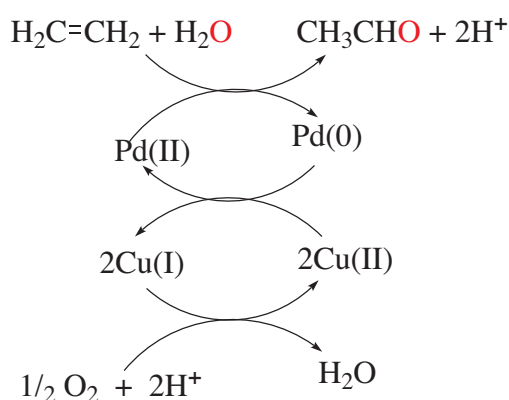
2. Catalytic conversion of Pd(0) to Pd(II) using  $CuCl_2$ .



3. The atmospheric oxidation of Cu(I) to Cu(II).



The above coupled reactions can be represented as shown below.

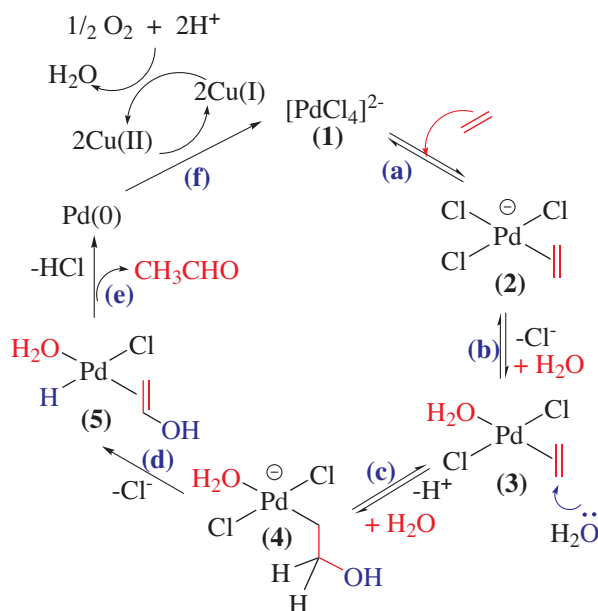


### Mechanism

The key step is the nucleophilic attack of a water molecule on the coordinated ethene. The mechanistic studies revealed the following rate equation for the process.

$$rate = k \frac{[PdCl_4^{2-}][C_2H_4]}{[Cl^-][H^+]}$$

$k$  is a constant. The rate of the reaction depends on the concentration of  $[PdCl_4]^{2-}$  and ethene. The rate is inversely proportional to the concentration of  $Cl^-$  and  $H^+$ . In the presence of chloride ions,  $PdCl_2$  exists in the form of  $[PdCl_4]^{2-}$ . It acts as the active catalyst for the conversion of  $CH_2=CH_2$  into  $CH_3CHO$  in the aqueous medium. A possible mechanism (catalytic cycle) is given in scheme 1.



Scheme 1. Proposed catalytic cycle

- Coordination of ethene with a loss of  $Cl^-$  to give (2)
- Coordination of  $H_2O$  with a loss of another  $Cl^-$  generates complex (3).
- External nucleophilic attack of water on the coordinated ethene with a loss of  $H^+$  to give anionic alkyl species (4).
- Slow step:  $\beta$ -H abstraction gives the coordinated enol of acetaldehyde
 
$$H_2C=CHOH \rightleftharpoons CH_3CHO$$
- Elimination of  $CH_3CHO$  and generation of Pd(0)

via the reductive elimination of HCl.

(f) Oxidation of Pd(0) to Pd(II) by Cu(II).

Note that the conversion of anionic complex (2) to a neutral complex (3) facilitates the nucleophilic attack of H<sub>2</sub>O on the coordinated ethene.

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