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.

$$H_2C{=}CH_2 \ + \ 1/_2\ O_2 \longrightarrow CH_3CHO$$

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

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

$$H_2C{=}CH_2 \ + \ PdCl_2 \ + \ H_2O \downarrow$$

$$CH_3CHO \ + \ Pd(0) \ + \ 2HCl$$

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

$$Pd(0) \ + \ 2CuCl_2 \downarrow$$

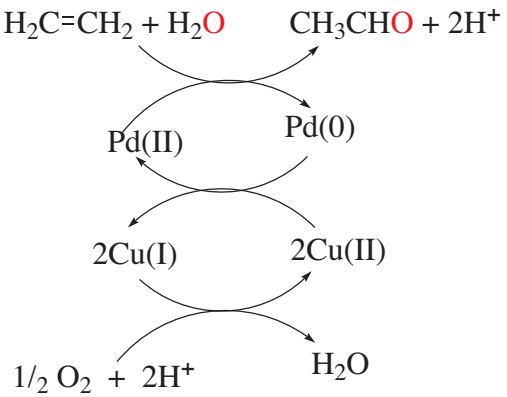
$$PdCl_2 \ + \ 2CuCl$$

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

$$2CuCl \ + \ 1/_2\ O_2 \ + \ 2HCl \downarrow$$

$$2CuCl_2 \ + \ H_2O$$

The above coupled reactions can be represented as shown below.

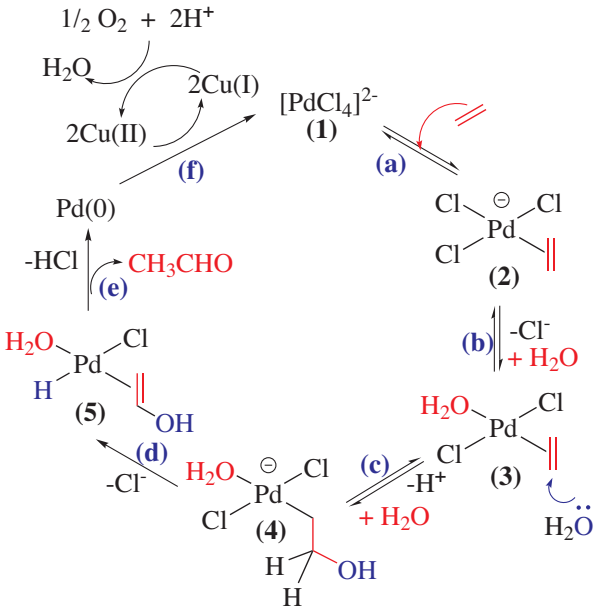


Mechanism

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

(a) Coordination of ethene with a loss of Cl^- to give (**2**)

(b) Coordination of H_2O with a loss of another Cl^- generates complex (**3**).

(c) External nucleophilic attack of water on the coordinated ethene with a loss of H^+ to give anionic alkyl species (**4**).

(d) Slow step: β-H abstraction gives the coordinated enol of acetaldehyde

$$H_2C{=}CHOH \rightleftharpoons CH_3CHO$$

(e) 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_2O on the coordinated ethene.

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