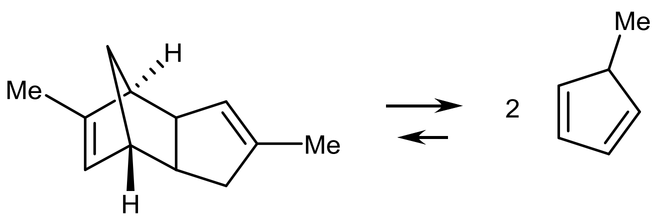
Analysis of T2 Incident Jacksonville Florida, December 2007

Methyl cyclopentadiene is produced from the corresponding dimer by thermal cracking. The anion is then generated by reaction with sodium – this generates hydrogen gas as a by-product. At T2 this was done in a single unit operation. $MnCl_2$ is then added and this quickly forms 1,1'-dimethyl-manganocene and sodium chloride. The addition of CO causes displacement of one of the π bonded ligands to give a sigma bonded complex which disproportionates with the final addition of the third CO ligand to give the Mn(I) product, methylcyclopentadienyl manganese tricarbonyl and a cyclopentadienyl radical. These radicals are very unstable and rapidly polymerise.

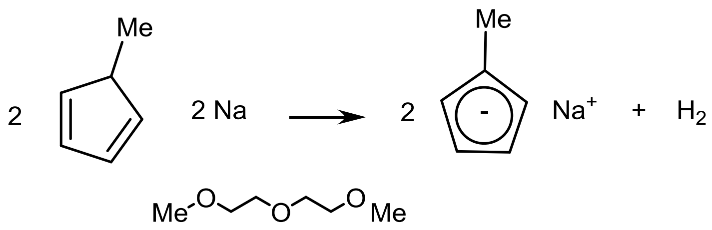
Looking in more detail at the individual steps[1]:

1) Cracking of methylcyclopentadiene dimer

This is an endothermic reaction which generates the monomer *via* a reverse Diels-Alder reaction, the typical cracking temperature is >150 °C. Most preparations of methylcyclopentadiene use 210 - 225 °C. The monomer is unstable and reactive. It can exothermically revert back to the more stable dimer *via* a Diels Alder reaction, or undergo a range of side reactions, especially polymerisation. Usually the monomer would be cooled at ~5 °C to stabilise before use.

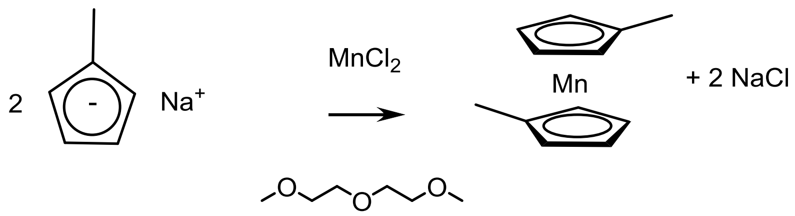


2) In the T2 process, the methylcyclopentadiene monomer is deprotonated *in situ* by molten sodium metal to generate the anion. This essentially removes the monomer from the equilibrium above. The salt is stable since the six-π electron anion is aromatic. The solvent is diglyme. The reaction is exothermic, normally run at 30 – 40 °C with cooling.

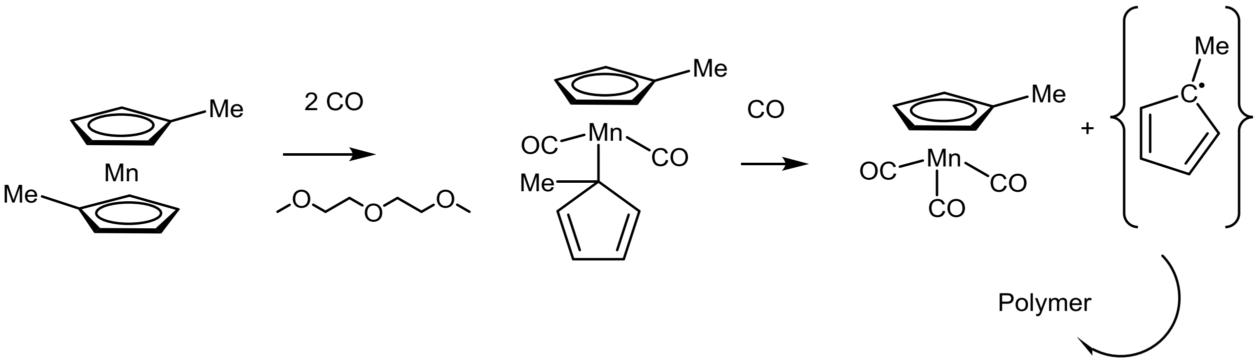


In the T2 process, this was run as a 'one pot' reaction in a single reactor.

3) Addition of manganous(II) chloride results in a methathetical reaction forming the sandwich compound 1,1'-dimethylmanganocene. This is essentially ligand exchange since there is no change in the Mn oxidation state.



4) Bubbling CO into the reaction results in a reduction of Mn(II) to Mn(I)



Questions: Part 1

Watch the following video from the US Chemical Safety and Hazard Investigation Board on the Reactive Chemical Explosion that happened at the T2 Laboratories **up to 5:05min**.

http://www.csb.gov/videos/runaway-explosion-at-t2-laboratories/

Then answer the following questions:

- **Considering the chemistry above, what hazards need to be handled in order to run the process safely?**
- **What are the merits of telescoping or 'one pot' reactions?**
- **In the case of the T2 process, was this a good or bad idea? Why?**
- **Ultimately, what do you think led to the uncontrolled reaction and explosion at T2?**

Questions: Part 2

Watch the remainder of the video from the US Chemical Safety and Hazard Investigation Board on the Reactive Chemical Explosion that happened at the T2 Laboratories **5:05min onwards.**

http://www.csb.gov/videos/runaway-explosion-at-t2-laboratories/

Then answer the following questions:

- **Given the same input chemicals, what would you do to make this process safer to run at scale?**
- **What chemicals could you substitute to make the process safer?**

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1. Investigation report T2 laboratories, http://www.csb.gov/assets/1/19/T2_Final_Copy_9_17_09.pdf, (accessed April 2016).