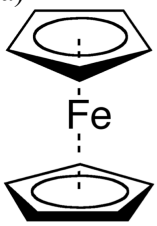
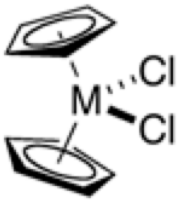
a) Describe the structure of ferrrocene.
b) How is this structure modified by the addition of substitutent groups (such as Cl) on the pentadiene rings?
c) Sketch the structure of a zirconia metallocene catalysts.
d) Explain the mechanism of polymerization using this zirconia catalysts
e) Are metallocenes heterogeneous or a homogeneous catalysts?

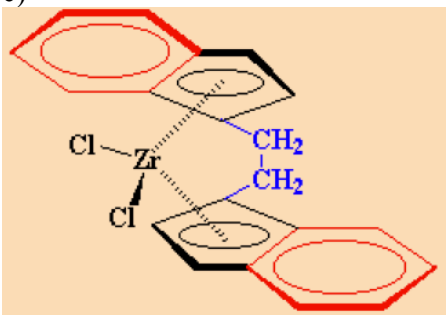
a)



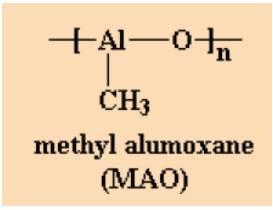
b) The two pentadiene rings will tilt with respect to each other allowing access to the caged metal atom for approaching chemical species.

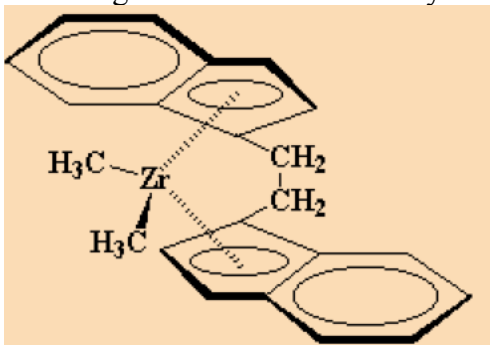


c)

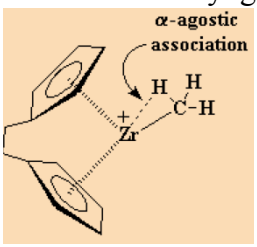


d) The molecule in part c is methylated through interaction with methyl alumoxane:

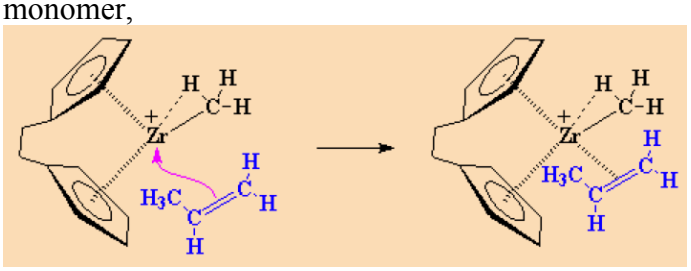




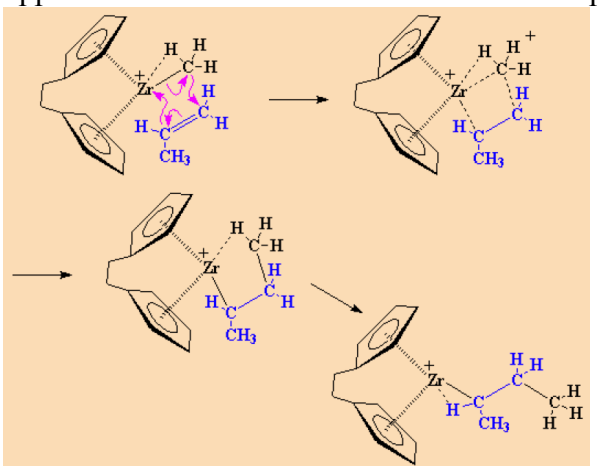
One labial methyl group leaves forming an α-agostic association,



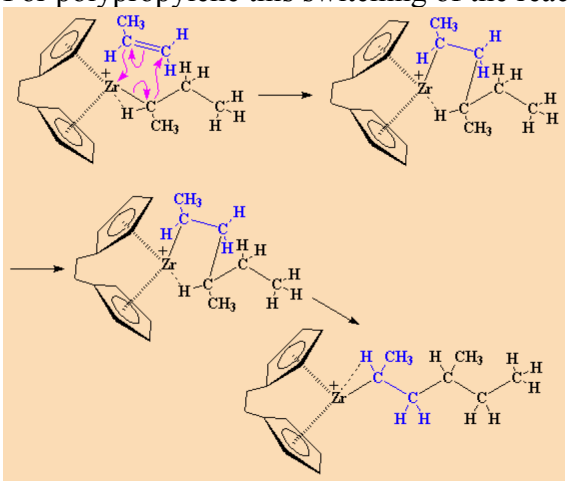
The positive charge on the zirconia atom associates with the unsaturated bond of an alkene monomer,



Rearrangement of the bonds leads to a 4 and then a 5 member cyclic structure that decomposes to the polymer chain allowing for a further a-agostic bond and the next monomer addition at the opposite side of the zirconia metallocene complex.



For polypropylene this switching of the reaction orientation leads to isotactic polymer,



e) Metallocenes are homogeneous catalysts.