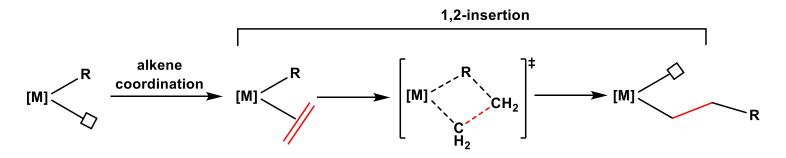
## Mechanism for Olefin Polymerization

## **Chain Propagation:**

- Cossee-Arlman Mechanism = good basic mechanism.
- Cossee et al. J. Catal. 1964, 3, 80 and 99.



- Brookhart-Green Mechanism = an improvement on the Cossee-Arlman mechanism  $\rightarrow$  it includes an  $\alpha$ -agostic interaction which helps to facilitate 1,2-insertion.
- Brookhart et al. J. Organomet. Chem. 1983, 250, 395.

$$[M] \xrightarrow{CH_2P} [M] \xrightarrow{H} [M] \xrightarrow{H} [M]$$

- Supporting calculations: Ziegler et al. Organometallics 2004, 104.
- Supporting experiments: Brintzinger et al. Angew. Chem., Int. Ed. 1990, 1412 (Zr), Piers and Bercaw J. Am. Chem. Soc. 1990, 9406.

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## **Chain Termination:**

• β-Hydrogen Transfer: H<sup>-</sup> transferred from the growing polymer chain to an incoming olefin. This is the dominant chain termination mechanism under the usual experimental conditions. Ziegler *et al. J. Am. Chem. Soc.* **1999**, 154.

$$[M] \xrightarrow{H_2} [M] \xrightarrow{H_2$$

•  $\beta$ -Hydrogen Elimination:  $\beta$ -hydrogen transferred to the metal. *ibid*.

$$[M] \xrightarrow{H}_{P} \qquad [M] \xrightarrow{H}_{P} \qquad [M] \xrightarrow{H}_{P}$$