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# Ab initio study on the impact of a mixed water-methanol feed on olefin formation during the MTO process

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In the methanol-to-olefin (MTO) process, an alternative for the depleting oil reserves, methanol is transformed into valuable base chemicals, catalyzed by zeolite or zeotype catalysts. In particular the chabazite structured H-SAPO-34 is of industrial interest due to its high selectivity to light olefins. [1] Studies on the MTO reaction mechanism led to the general acceptance of the hydrocarbon pool (HP) mechanism governing the MTO process, where an organic compound trapped in the catalyst acts as a co-catalyst. [2] Polymethylbenzenes are identified as dominant HP species in H-SAPO-34 [3], for which the side-chain and paring mechanism are the proposed reaction cycles represented in Figure 1.

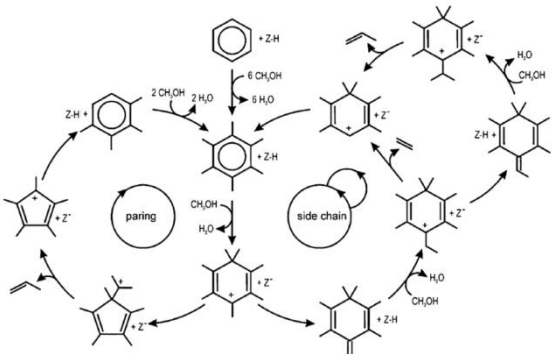


**Figure 1.** Schematic representation of the reaction mechanisms proposed for the MTO process with aromatics as HP species.

Due to future use of biomass feedstock, containing high amounts of water, the influence of water in the methanol feed on the MTO process is relevant. Experimental research already showed a reduced coking rate and increased selectivity to light olefins due to water addition. [4] Earlier dynamic simulations investigated the adsorption behavior of water in H-SAPO-34 [5], but the water influence on the MTO reaction mechanism is still unclear. Therefore, this study investigates the effect of water on elementary steps of the proposed mechanisms using advanced molecular dynamics techniques, which are able to mimick operating conditions.

**References**

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