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A density functional theory study of oxidation of benzene to phenol by N_2O on Fe- and Co-ZSM-5 clusters

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Abstract: Density functional theory (DFT) calculations were carried out in the study of oxidation of benzene to phenol by N_2O on relaxed [$(SiH_3)_4AlO_4M$] (where M=Fe, Co) cluster models representing Fe- and Co-ZSM-5 surfaces. The catalytic cycle steps are completed for both Fe-ZSM-5 and Co-ZSM-5 clusters. The general trend of the results that were obtained in terms of activation barriers for the Fe-ZSM-5 cluster is in agreement with the experimental and theoretical literature. It was observed that the phenol formation step is the rate-limiting step for both clusters and Co-ZSM-5 surface has a lower activation barrier than the Fe-ZSM-5 surface (i.e. 35.82 kcal/mol vs. 45.59 kcal/mol, respectively).

Key Words: DFT, benzene oxidation, phenol, N_2O, Fe-ZSM-5, Co-ZSM-5.

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