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## QUANTUM MECHANISTIC STUDIES OF THE OXIDATION OF ETHYLENE USING GROUP VII B OXO COMPLEXES.

Transition-metal-mediated oxygen transfer reactions are of great importance in both industry and academia; thus, a series of group VII B oxo complexes of the type  $MO_3L$  ( $L = O^-$ ,  $F^-$ ) and their effects as oxidation catalysts on ethylene have been studied on the singlet and triplet PES at the DFT B3LYP/LACVP\* level of theory. Molecular structures were stable on the singlet reaction surface except for dioxomangana-2,5-dioxolane intermediate formation where the triplet structure was stable. Frontier molecular orbital calculations showed that the highest occupied molecular orbital of ethylene molecule bonds to the lowest occupied molecular orbital of the metal-oxo catalysts except for  $MO_3L$  ( $M = Re, Tc, Mn$ , and  $L = O^-$ ) complexes where the vice versa occurs. Dioxylation along the [3+2] addition route on the singlet reaction surface using  $ReO_3L$ ,  $TcO_3L$ , and  $MnO_3L$  ( $L = O^-$ , and  $F^-$ ) catalysts are stable as compared to the [2+2] pathway. The rearrangement of the metallaoxetane intermediate to the dioxylate is not a feasible reaction for all the catalytic pathways studied except in the case of the perrhenate catalyzed pathway.

The formation of epoxides on the singlet surface is kinetically favorable through the [2+1] channel for the  $MnO_3L$  ( $L = F^-$ ) catalyzed pathway over the epoxide formation via the [2+2] route whereas epoxide formation occurs via the [2+2] pathway for the  $ReO_3F$  and  $TcO_3F$  catalyzed pathway. The  $MnO_3L$  complexes showed the highest polarity followed by the  $TcO_3L$  and  $ReO_3L$  complexes.

The pertechnetate and perrhenate catalyzed surfaces form exclusively diols but due to their endergonic nature and the high activation barrier, diol formation from these catalysts will be hindered. Also, dioxylation strength decreases from Mn complexes to Re complexes on the singlet PES.

$MnO_4^-$  (singlet) is the best catalyst for the exclusive formation of the diols whereas the best exclusive epoxidation catalyst among all the complexes is  $MnO_3F$  (singlet) complex.

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