

Theoretical Study of Ethylene Addition to $O=W(=CH_2)(CH_3)_2$

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Dedicated to Prof. Helgard G. Raubenheimer on the occasion of his 65th birthday

Quantum chemical calculations using density functional theory at the B3LYP level of theory were carried out to investigate the reaction pathways for the addition of ethylene to $WO(CH_3)_2(CH_2)$ (**W1**). The results are compared to those of previous theoretical studies of the ethylene addition to $OsO_3(CH_2)$ (**Os1**) and $ReO_2(CH_3)(CH_2)$ (**Re1**). The theoretically predicted reactions pathways exhibit significant differences. The energetically most favourable reaction of the tungsten system **W1** is the $[2+2]_{W,C}$ addition across the $W=C$ double bond yielding the metallacyclobutane **W3a** which then rearranges to the slightly more stable isomer **W3b**. The $[2+2]_{Re,C}$ addition of the rhenium compound yielding the metallacyclobutane **Re3a** has the lowest activation barrier for the ethylene addition to the rhenium system, but the reaction is endothermic while the exothermic formation of the more stable isomer **Re3b** has a much higher activation barrier. The $[3+2]_{C,O}$ addition **Os1** + $C_2H_4 \rightarrow$ **Os2** is the thermodynamically most favorable reaction of the osmium compound.

Key words: Reaction Mechanism, DFT Calculations, Oxo Carbene Complexes, Cycloaddition, Metallacycle