# $\mathrm{Mo}\left(\mathrm{OSi}(\mathrm{tBu})_{3}\right)_{3}$ : Structure and Reactivity 

M. Pucino ${ }^{1}$, F. Allouche ${ }^{1}$, M. Wörle ${ }^{2}$, C. Copéret ${ }^{1 *}$<br>${ }^{1}$ ETH Zurich, ${ }^{2}$ ETH Zürich

Cr (III) surface species, prepared from Cr (III) siloxide molecular precursor, are highly active catalysts for olefin polymerization and alkane dehydrogenation. ${ }^{1,2}$ We have thus become interested in generating low coordinated isoelectronic Mo (III) surface to investigate their corresponding reactivity. To date, low coordinate Mo (III) compounds are rare; they typical require large somewhat rigid ligands like in $\mathrm{Mo}[\mathrm{N}(\mathrm{R}) \mathrm{Ar}]_{3} \quad\left(\mathrm{R}=\mathrm{tBu}, \mathrm{Ar}=3,5-\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{Me}_{2}\right)^{2}$ and $\mathrm{Mo}\left(\mathrm{OSi}{ }^{\mathrm{t}} \mathrm{Bu}\right)_{3} \cdot{ }^{3}$ Here, we have developed the synthesis of $\mathrm{Mo}\left(\mathrm{OSi}(\mathrm{OtBu})_{3}\right)_{3}(\mathbf{1})$ and investigated its reactivity towards a broad range of small molecules $\left(\mathrm{CO}_{x}, \mathrm{~N}_{2} \mathrm{O}, \mathrm{O}_{2}, \mathrm{~S}_{8}\right.$, ethylene and $\left.\mathrm{N}_{2}\right)$. The complex 1 has three siloxy ligands adopting a $\mathrm{k}^{2}$-coordination, yielding an overall distorted octahedral geometry. This complex reacts at room temperature with $\mathrm{N}_{2}$ to give the corresponding Mo (VI)-nitrido compound by dinitrogen splitting via $[\mathrm{Mo}=\mathrm{N}=\mathrm{N}=\mathrm{Mo}$ ] intermediate, which was isolated at low temperature and fully characterized. This complex also react with $\mathrm{N}_{2} \mathrm{O}$, but does not lead to the splitting of $\mathrm{N}-\mathrm{O}$ bond as expected from metal mediated decomposition of nitrous oxide ${ }^{4}$, but rather of $\mathrm{N}-\mathrm{N}$ bond, leading to [ $\mathrm{Mo}-\mathrm{h}^{1}-\mathrm{NO}$ ] with NO in linear fashion and $\mathrm{Mo}(\mathrm{VI})-\mathrm{N}$. Similarly, reaction with $\mathrm{CO}_{2}$ yields $\mathrm{Mo}(\mathrm{III})-\mathrm{CO}$ and $\mathrm{Mo}(\mathrm{V})-\mathrm{O}$. The former can also be obtained from the reaction of $\mathbf{1}$ with CO. Reaction of $\mathbf{1}$ with $\mathrm{S}_{8}$ yields $\mathrm{Mo}(\mathrm{V})$-S complex. Finally, the reaction of $\mathbf{1}$ and ethylene generates the corresponding $p$-complex as it does by reaction with 2-butyne.

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