18.5-4 MOLECULAR ANALOGUES OF SURFACE COMPLEXES AND MODELIZATION OF METAL-SUPPORT INTERACTION: X-RAY STRUCTURE OF $(\mu\text{-H})(\mu\text{-OSiEt}_3)\text{Os}_3(\text{CO})_{10}$, COMPUTER MODELED SURFACE STRUCTURES $(\mu\text{-H})(\mu\text{-OSi}\equiv)\text{Os}_3(\text{CO})_{10}$ AND $(\mu\text{-OSi}\equiv)_2\text{Os}_3(\text{CO})_{10}$. By Leh-Yeh Hsu and Sheldon Shore, Department of Chemistry, The Ohio State University Columbus, Ohio 43210, U.S.A., and Lindora D'Ornelas, Agnes Choplin and Jean-Marie Basset, Institut de Recherches sur la Catalyse, Laboratoire Propre du C.N.R.S., CONVENTIONNE A l'Universite Claude Bernard, Lyon I, France.

Reaction between $\text{Os}_3(\text{CO})_{12}$ and silica results in a new species which is believed to be the surface cluster. Suggestions for this surface structure have been based on various experimental techniques. Two models have been considered: 1)a single surface oxygen binding the triosmium cluster by bridging two Os atoms, $(\mu\text{-H})(\mu\text{-OSi}\equiv)\text{Os}_3(\text{CO})_{10}$, I, 2)two surface oxygens bridging the same two osmiums, $(\mu\text{-OSi}\equiv)_2\text{Os}_3(\text{CO})_{10}$, II. In order to have a better understanding of the real structure of the surface cluster, the crystal structure of $(\mu\text{-H})(\mu\text{-OSiEt}_3)\text{Os}_3(\text{CO})_{10}$, III, has been determined. The molecule consists of an Os_3 isoceles triangle with a bridge hydrogen and a bridge OSiEt_3 group between two Os. Each of these osmium atoms is also bound to three terminal carbonyl groups. The third Os atom is bound to four terminal carbonyl groups. The infrared data for I and III are very similar which suggests that I adopts on the silica surface the same type of bonding as III. Computer models of the surface complexes I and II by grafting III and $(\mu\text{-OMe})_2\text{Os}_3(\text{CO})_{10}$, IV, on an ideal 100 plane of β-cristobalite fully covered with hydroxyl groups and partially dehydrated were derived using CHEMX and MacroModel systems. The cluster III can not be accomodated either on the fully hydroxylated or partially hydroxylated 100 face of β-cristobalite. The best way to accomodate the cluster without any steric contraints was achieved when the cluster was grafted to the edge obtained from the interception of the 100 and 010 faces. The cluster IV could not be accomodated either on the 100 face or edges and corners.