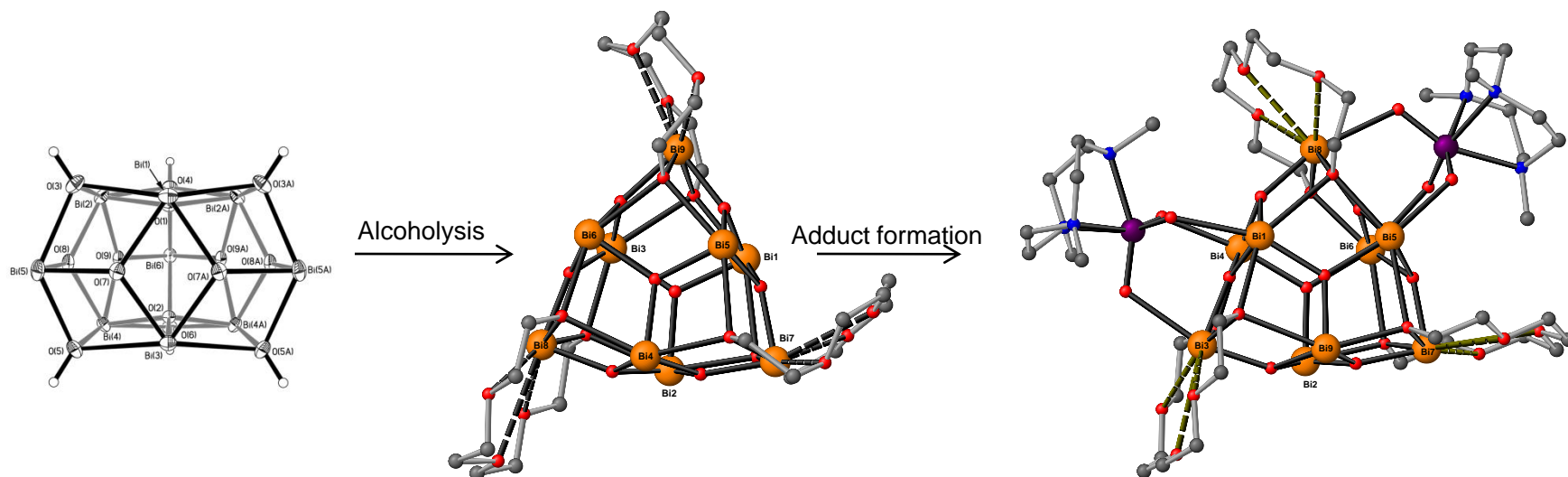


Molecular Models for Bi/Mo Oxidation Catalysts

John H. Thurston, Department of Chemistry, The College of Idaho

The SOHIO process remains one of the most important routes for the conversion of propene into acrolein and acrylonitrile on an industrial scale. Despite the importance of this process, the mechanism for the observed transformations remains, at best, poorly understood.

Our group has attempted to develop molecular models of the commercially used SOHIO catalyst as a route to more completely explore the chemistry of this system. In the course of this project, we have attempted to target complexes whose spatial arrangement and bonding parameters are reflective of what is seen in the bulk material. In so doing, we have developed a novel “bottom-up” synthetic route to the formation of high nuclearity heterobimetallic coordination complexes that contain bismuth and either molybdenum or tungsten through direct Lewis acid-base adduct formation. The complexes formed in this manner show excellent stability in the solid state and in solution. We have successfully tailored the composition of the stabilizing organic framework to include functional groups that are implicated in some of the key steps of the proposed SOHIO cycle, including amine and allyl moieties. Future work on this system will be directed toward assessing the chemistry at the transition metal center in these coordination complexes, as well as developing new species that contain more reactive ligand sets.



In the image above, Bi atoms are orange and Mo atoms are purple