In this research, we are pursuing a combined computational and experimental study of enantioselective Rh-catalyzed hydrogenation of acrylic acid derivatives. The specific aim of this work is to develop a protocol for the virtual screening of chiral ligand libraries to predict the % e.e.'s for given substrate/catalyst combinations to assist in the selection and/or design of catalysts for experimental use. The animation that is provided here depicts one of the pathways that we have investigated computationally for acrylamide hydrogenation. A Rh phosphine complex is shown interacting with the acrylamide substrate through formation of a Rh-oxygen bond and pi-complexation with the olefinic double bond. As molecular hydrogen approaches from the top, the H-Rh bond order increases as the H-H bond weakens in a square planar transition state (SQPL-TS). A molecular hydrogen (MOLH2) complex is formed, which then proceeds to the dihydride (DIHY) complex. One hydrogen first migrates to the beta carbon through a high energy DIHY-TS followed by transfer of the second hydrogen to the alpha carbon via the alkylmetal hydride transition state (ALHY-TS).