Computational studies of small neutral vanadium oxide clusters and their reactions with sulfur dioxide

ELENA JAKUBIKOVA, SHENG-GUI HE, YAN XIE, Colorado State University, Department of Chemistry, YOSHIYUKI MATSUDA, Tohoku University, Department of Chemistry, ELLIOT BERNSTEIN, Colorado State University, Department of Chemistry — Vanadium oxide is a catalytic system that plays an important role in the conversion of SO$_2$ to SO$_3$. Density functional theory at the BPW91/LANL2DZ level is employed to obtain structures of VO$_y$ (y=1, . . . ,5), V$_2$O$_y$ (y=2, . . . ,7), V$_3$O$_y$ (y=4, . . . ,9), V$_4$O$_y$ (y=7, . . . ,12) and their complexes with SO$_2$. BPW91/LANL2DZ is insufficient to describe properly relative V-O and S-O bond strengths of vanadium and sulfur oxides. Calibration of theoretical results with experimental data is necessary to compute enthalpies of reactions between V$_x$O$_y$ and SO$_2$. Theoretical results indicate SO$_2$ to SO conversion occurs for oxygen-deficient clusters and SO$_2$ to SO$_3$ conversion occurs for oxygen-rich clusters. Subsequent experimental studies confirm the presence of SO in the molecular beam as well as the presence of V$_x$O$_y$ complexes with SO$_2$. Some possible mechanisms for SO$_3$ formation and catalyst regeneration for solids are also suggested.