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 \(\text{VO}_y\) (\(y=1, \ldots, 5\)), \(\text{V}_2\text{O}_y\) (\(y=2, \ldots, 7\)), \(\text{V}_3\text{O}_y\) (\(y=4, \ldots, 9\)), \(\text{V}_4\text{O}_y\) (\(y=7, \ldots, 12\)) 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 \(\text{V}_x\text{O}_y\) 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 \(\text{V}_x\text{O}_y\) complexes with SO\(_2\). Some possible mechanisms for SO\(_3\) formation and catalyst regeneration for solids are also suggested.

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