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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 Stete 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_2O_y (y=2,...,7), V_3O_y (y=4,...,9), V_4O_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_xO_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_xO_y complexes with SO_2. Some possible mechanisms for SO_3 formation and catalyst regeneration for solids are also suggested.

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