

Abstract Submitted
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Cooperative Effects in the Oxidation of CO by Palladium Oxide Cations¹ ARTHUR C. REBER, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, ERIC C. TYO, CHRISTOPHER L. HARMON, A. WELFORD CASTLEMAN JR., Departments of Chemistry and Physics, Penn. State University — It is shown that cooperative reactivity plays an important role in the oxidation of CO to CO₂ by palladium oxide cations. Comprehensive studies including guided-ion-beam mass spectrometry and theoretical investigations reveal the reaction products and profiles of PdO₂⁺ and PdO₃⁺ with CO through oxygen radical centers and dioxygen complexes bound to the Pd atom. We find that the O radical centers are more reactive than the dioxygen complexes, and experimental evidence of both direct and cooperative CO oxidation with the adsorption of two CO molecules are observed. The binding of multiple electron withdrawing CO molecules is found to increase the barrier heights for reactivity due to decreased binding of the secondary CO molecule, however reactivity is enhanced by the increase in kinetic energy available to hurdle the barrier. We examine the effect of oxygen sites, cooperative ligands, and spin including two-state reactivity.

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