

ATOMIC CATIONS: THE ULTIMATE SITES FOR CATALYSIS

Diethard K. Böhme

Department of Chemistry and Centre for Research in Mass Spectrometry,

York University, Toronto, Ontario, Canada M3J 1P3

Nature's gifts to atomic ions include a chemical affinity for atoms and molecules and a charge that allows long-range electrostatic interactions with molecules. As a consequence, chemical reactions between ions and molecules can provide fast alternative routes to slow chemical transformations between neutral molecules. This will be illustrated, using both experiment and theory, with examples of "atom transport" and "bond activation" catalysis. The experimental approach involves use of an Inductively-Coupled Plasma/Selected-Ion Flow Tube tandem mass spectrometer (ICP/SIFT/Q) that has allowed us to probe the catalytic properties of up to 59 atomic ions on the periodic table. Thermodynamic criteria for atomic-ion catalysis provide a "window of opportunity" for catalysts that is refined by the kinetic results. We also propose a new measure of catalytic efficiency. Emphasis will be given to the catalytic reduction of nitrogen oxides and the oxidation of hydrogen and several small hydrocarbons.

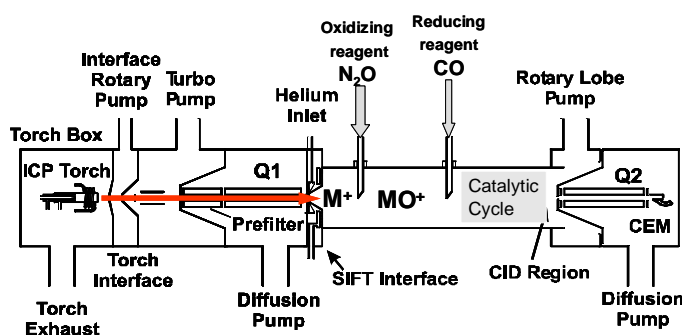


Fig. 1. Schematic view of ICP/SIFT/Q instrument.

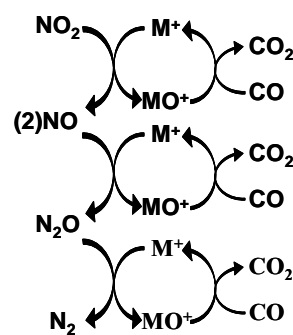


Fig. 2. Coupled 3-cycle catalytic reduction of NO₂ by CO.

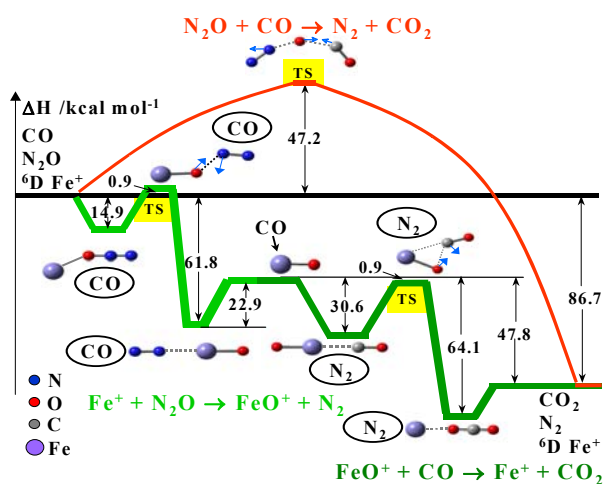


Fig. 3. Potential-energy landscape for the reduction of N₂O by CO catalyzed by iron cations.