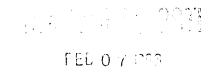


•



Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE GAS-PHASE OXIDATION OF ATOMIC BORON AND BORON MONOXIDE

LA-UR--86-262

DE86 006028

AUTHOR(S) Richard C. Oldenborg, CHM-4 Steven L. Baughcum, CHM-4

SUBMITTED TO. Proceedings of the First International Laser Science Conference American Institute of Physics Dallax, TX, November 1985

# DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect these of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce - the published form of this contribution, or to allow others to do so, for U.S. Government purposes

The Los Alamos National Laboratory requests that the publisher identity this article as work performed under the auspices of the U.S. Department of Energy



SALAMOS Los Alamos National Laboratory Los Alamos, New Mexico 87545

### GAS-PHASE OXIDATION OF ATOMIC BORON AND BORON MONOXIDE

## Richard C. Oldenborg and Steven L. Baughcum Chemistry Division Los Alamos National Laboratory Los Alamos, New Mexico 87545

## ABSTRACT

Rate constants for the reactions of  $B + O_2$  and  $BO + O_2$  have been measured over the temperature range 298-1180 K using the laser photolysis/laser-induced fluorescence technique. The rate of the  $B + O_2$  reaction increases slightly with increasing temperature. In contrast, the  $BO + O_2$  reaction has a negative temperature dependence and is believed to proceed via a stable intermediate complex.

#### INTRODUCTION

The emphasis in much of the previous boron slurry rocket fuel research has been on particle ignition, yet roughly half of the potential energy content of boron fuels is released in the gas-phase oxidation of BO(g) to  $B_2O_3(g)$ . We are investigating the kinetics of the key gas-phase boron oxidation reactions over a wide temperature range so that a comprehensive reaction scheme can be assembled and evaluated. Our initial effort has concentrated on the BO +  $O_2$  +  $BO_2$  + O reaction, which is considered to be the key BO oxidation step in dry atmospheres.

#### EXPERIMENTAL

Volatile boron compounds such as  $BCl_3$  are photolyzed with an excimer laser to provide an essentially instantaneous source of boron atoms. These quickly react with  $O_2$  to yield BO molecules,

$$B + 0_2 + B0 + 0$$

which in turn react with additional  $0_{2}$  to produce  $BO_{2}$ .

$$BO + O_2 + BO_2 + O$$

The time histories of the B, BO, and BO<sub>2</sub> are monitored using laser-induced fluorescence (LIF) and chemiluminescent techniques.

Systematic variation of  $0_2$  pressure yields the desired rate constants. Experiments are conducted in a high-temperature cell capable of 298-1500 K operation. All experiments are in an argon diluent at 25 torr total pressure.

## **RESULTS AND DISCUSSION**

The B +  $O_2$  reaction rate constant was measured to be 7 x 10<sup>-11</sup> cc/molecule-s at 298 K and increases slightly with increasing temperature. In contrast, the BO +  $O_2$  reaction rate constant is somewhat slower at 298 K, i.e., 2 x 10<sup>-11</sup> cc/ molecule-s, and decreases with increasing temperature in a non-Arrhenius fashion. The reaction may proceed via a stable BO<sub>3</sub> intermediate

$$BO + O_2 \xrightarrow{\rightarrow} BO_3 \xrightarrow{\rightarrow} BO_2 + O$$
,

which may help account for this interesting temperature dependence. Expariments are in progress to better establish the functional form of this temperature dependence and to test the role of third-body collisions at both high and low gas pressures. Other key boron oxidation reactions are also presently under investigation.

## ACKNOWLEDGMENTS

The technical assistance of Kenneth Winn of Los Alamos National Laboratory is gratefully acknowledged. The work is supported by the Air Force Office of Scientific Research (AFOSR).