NATIONAL BUREAU OF STANDARDS REPORT

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FINAL REPORT

ENERGY DISTRIBUTIONS OF OH IN H_2-O_2 FLAMES

by

H. P. Broida

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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NBS PROJECT		NBS REPORT
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ENERGY DISTRIBUTIONS OF OH IN H_2-O_2 FLAMES

by

H. P. Broida
Temperature Measurements Section
Division of Heat and Power

Project NR-051-303 (Government Order NAonr-136-523)
and Project NR-019-129 (Contract N-ONR-737)

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BACKGROUND

Early in 1952, under Projects NR-051-303 and NR-019-129, the National Bureau of Standards and Hydrocarbon Research, Inc. engaged in a joint theoretical and experimental investigation of the distribution of vibrational and rotational energies of hydroxyl radicals in hydrogen-oxygen flames. Calculations were to be made of the transition probabilities from initial states of the reactants to final states of the products in the chemical reactions

$$H_2 + O \longrightarrow OH + H$$

$$O_2 + H \longrightarrow OH + O$$

Measurements of OH distributions in flames were to be made in order to assist in the choice of range of parameters and to check the final predictions. It was hoped that these studies would contribute to the basic understanding of general combustion problems and would advance methods of calculations of properties of flames so that theory could guide future experiments and practical applications.

The project was terminated at the end of the fiscal year 1953 due to the lack of additional funds. At that time, less than 60% of the originally estimated time and funds had been used.

TECHNICAL PROGRESS REPORT AND STATUS

At the outset the work had been divided into three interrelated phases which were carried out by three separate groups.

(1) The adaptation of Golden's general quantum mechanical theory of reaction rates (S. Golden, J. Chem. Phys. 17, 621 [1949]) to a form suitable for calculation on large scale automatic computing machinery was completed at Hydrocarbon Research, Inc. (Project NR-019-1299). This work was summarized in a report, "A Quantum Mechanical Model for Use by SEAC in the Calculation of Chemical Transition Probabilities," by A. M. Peiser and S. Golden, February 27, 1953.

(2) The computation of selected transition probabilities was the responsibility of the Computation Laboratory at the National Bureau of Standards (Project NR-051-303). A code developed for carrying out these computations on SEAC, the National Bureau of Standards' automatic computer, and the preliminary test of two computations on SEAC has been described by A. N. Gleyzal, "Computation of Chemical Transition Probabilities," NBS Report 3275, April 29, 1954.

(3) Experimental work relating to the choice of parameters for the computations and the construction of equipment for experimental verification of the calculated results was carried out in the High Temperature Program at the National Bureau of Standards, primarily without ONR support. These investigations have been reported in the literature (e.g. J. Chem. Phys. 20, H. P. Broida and G. T. Lalos, 1466-71 (1952); 21, W. R. Kane and H. P. Broida, 347-54 (1953); and 21, H. P. Broida, 1165-69 (1953).

Additional apparatus for measurement of OH distributions under conditions approximately described by the computations has recently been completed. This equipment consists of (1) a burner suitable for sustaining a flame of pre-mixed hydrogen and oxygen at pressures below 3 mm Hg, (2) a high intensity ultra-violet light source suitable for precision OH absorption measurements and (3) the extension to the infra-red of a previously available high resolution ultra-violet and visible monochromator.

CONCLUSIONS

Briefly stated, the work has not gone far enough to permit any positive statement about the success or failure of this attempt to provide a combined theoretical and experimental treatment of the energy distribution of OH in flames. The positive results are:

(1) There has been neither theoretical nor experimental evidence to indicate that the proposed calculations and experimental verification could not be carried out.

(2) The SEAC can do the computations for a selected chemical reaction and temperature in the order of 125 hours (it has been estimated that perhaps 300 years would be required for hand calculation).

(3) Apparatus and techniques are available for measuring OH distributions in flames for comparison with calculated predictions.

RECOMMENDATIONS

In view of the progress made to date at a rate somewhat less than originally estimated and since no evidence of error has been found in the assumptions upon which this program was started, the following recommendations are made:

(1) That Dr. S. Golden (now at Brandeis University) be encouraged and supported to review the progress to date, the details of the code prepared for SEAC, and the overall problem with the aim of determining whether the work should be extended or concluded.

(2) (Providing Dr. Golden approves) That the present or modified code be used to compute the transition probabilities for OH in various rotation and vibration states from the reaction

$$O_2 + H \longrightarrow OH + O$$

at temperatures of 2500°K and 1000°K. The 250-300 hours required for these computations would cost approximately $8,000.

(3) That an experimental investigation of the rotational and vibrational intensity distributions of OH in hydrogen-oxygen flames be made at low pressures to determine the degree to which such distributions are not consistent with equilibrium distributions.

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