CATALYSIS

Progress in Research

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PREFACE

This conference on Catalysis was held under the auspices of the NATO Science Committee as part of its continuing effort to promote the useful progress of science through international cooperation.

The Science Committee Conferences are deliberately designed and structured to focus expert attention on what is not known, rather than what is known. The participants are carefully selected to bring together a variety of complementary viewpoints. Through intensive group discussion, they seek to reach agreement on conclusions and recommendations for future research which will be of value to the scientific community.

We believe that the endeavour has been particularly successful in the present case. Some twenty-five papers, either in the form of reprints or specially written reviews were contributed by the participants for advance circulation, to outline the state-of-the art in the three areas of heterogeneous, homogeneous and metalloenzyme catalysis and to focus attention on key problems. The availability of this background material precluded the need for lengthy introductory presentations and permitted rapid initiation of interdisciplinary discussions. All participants gave generously and enthusiastically of their expertise and effort during the week of the meeting, often long past normal bedtime hours, and we extend to them our deep gratitude.

We are delighted to have this opportunity to record our special thanks to Professor Fred Basolo and Robert Burwell for their diligent efforts as Chairman and Co-Chairman of the meeting, to their colleagues on the Organizing Committee, Professors S. Benkovic, J. Chatt, C. Kemball, R. Ugo and V. Ullrich, for their wise guidance, and to the leaders and recorders of the Working Groups, as listed, for their indispensable dedication. The assistance of Professor R. Lontie in preliminary editing of this volume is gratefully acknowledged.

We also wish to record our appreciation to the US Office of Naval Research, which contributed significantly to the success of the meeting through provision of logistic support.

Eugene G. Kovach
Deputy Assistant Secretary General for Scientific Affairs

INTRODUCTION

The desirability of classifying problems and accelerating their solution in the general area defined as catalysis has become apparent to many within the scientific community. The field concerned with catalysis can be generally divided into three specialities which encompass enzymatic, heterogeneous, and homogeneous reactions.

Heterogeneous catalysis is still the basis of most commercial chemical processes and therefore is the subject of extensive investigation within industry. Although homogeneous catalysis has not gained a similar state of commercial importance, basic research on many of the mechanisms is in progress. The third area, enzymatic catalysis, has developed rather independently mainly through the efforts of biochemists and biophysicists.

Although rapid progress in all three specialities is evident, it is also obvious that significant developments within one have not always been recognized for their pertinence to another. It was the intent of the Organizing Committee, therefore, to assemble a group of active scientists knowledgeable in contemporary theory and experimental design within their respective specialities to foster a mutually beneficial exchange of information. Such communication might particularly lead to recognition of problems that are truly interdisciplinary in scope and also to proposed solutions for these problems.

To enhance the degree of interaction six topics, "Kinetics and Mechanism" "Hydrogenation/Dehydrogenation", "Nitrogen Fixation", "Oxygen Activation" "Hydrocarbon Activation" and "Heterogenizing Catalysts", were chosen for discussion, based mainly on the judgement of the Organizing Committee that the probability for overlap between the above three specialities was maximal for these subjects. It is emphasized that these topics served merely as a framework for discussion and were neither all inclusive nor representative of other equally important problems within the field of catalysis. The resulting reports were produced during three days of intensive discussion within small groups that followed a short period of general introduction to

acquaint all with the semantics and present status of research within the three subdivisions of catalysis.

By the nature of the structure of the conference, no *systematic* consideration was given to the problems which lie within just one of the areas of catalysis nor to overlap between any of these areas and external areas—for example, between enzyme catalysis and microbiology, or between heterogeneous catalysis and surface chemical physics. Furthermore, the overlap between metallo-enzymes and organometallic chemistry was considered extensively but many aspects of coordination chemistry potentially useful for catalysis of such reactions as hydrolysis, transamination, decarboxylation, etc., received little attention. Thus, the conclusions of the conference do not extend to aspects primarily within each speciality nor to overlaps between any one area and adjacent non-catalytic areas.

It was impossible within the allotted time period to correct imbalance as to the length of individual reports of the six working groups. Such differences should not be construed as reflecting the relative importance or priority to be assigned a given topic, but simply as a consequence of the inequality in topic scope and the heterogeneity of the groups involved. It seemed preferable to reproduce the group reports without attempting to edit them or reduce them to a uniform format as this might have destroyed their originality. Instances of repetition function to pinpoint problems, techniques, and recommendations which are truly interdisciplinary. The references at the end of the Group Reports are intended to give the reader a general guide to further information on the subject.

The present volume includes, in addition to the Group Reports, specially commissioned papers reflecting the current situation on key aspects of catalysis research. This mixing of scientists from related but not identical disciplines led to an enthusiastic articulation of potential problem areas, present deficiencies and self-criticism within and without their own areas of speciality. The Conclusions (Page 187) attempt to summarize the findings of the Working Groups, but a close reading of the Group Reports as well is strongly urged.

The Organizing Committee

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