MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963
SYNTHETIC STUDIES WITH METALLOCARBORANES

FINAL TECHNICAL REPORT, 15 Dec 71-14 Dec 74

Principal Investigator: M. F. Hawthorne

15 December 1971 to 14 December 1974

ARO(D) Grant No. DA-ARO-D-31-124-72-G63

Department of Chemistry
The University of California
Los Angeles, California

Approved for Public Release;
Distribution Unlimited.
During the contract period major advances along several related lines of research were made.

The polyhedral expansion reaction of carboranes was extended to 8, 9, 10 and 11 vertex species yielding the respective 9, 10, 11 and 12 vertex metallocarboranes of both cobalt and iron. This reaction was also useful in producing bimetallic metallocarboranes. Bimetallic and trimetallic metallocarboranes were also produced in the expansion of monometallocarboranes.

The reaction of nucleophiles with metallocarboranes produced high yields of novel Lewis base adducts of nido metallocarboranes. Thermal reactions of metallocarboranes, including migration of cobalt and carbon atoms and thermal metal transfer reactions were thoroughly explored and general rules governing these reactions were proposed. In addition, electron counting rules for metallocarboranes were proposed, defining electronic considerations for stable closo and nido species.

X-ray diffraction studies of several important metallocarboranes were performed confirming proposed structures for these species.
PUBLICATIONS


The following scientific personnel were supported by this project during this reporting period:

William J. Evans, Ph.D., 1973
Frederick Lo, Graduate Student
James A. Doi, Graduate Student
Dr. C. J. Jones, Postdoctorate
Dr. Donald F. Dustin, Postdoctorate
Dr. William T. Scroggins, Postdoctorate

Respectfully submitted,

M. F. Hawthorne
April 16, 1975
SYNTHETIC STUDIES WITH METALLOCARBORANES

M. F. Hawthorne

Department of Chemistry
University of California, Los Angeles
Los Angeles, California 90024

U. S. Army Research Office
Box CH, Duke Station
Durham, North Carolina 27706

REPORT DATE
April 18, 1975

M. F. Hawthorne

Approved for public release; distribution unlimited.

Metallocarboranes, Polyhedral expansion, cobaltacarboranes, ferracarboranes, cobaltaferracarboranes, X-ray diffraction.

The syntheses of mono-, bi- and tri-metallic metallocarboranes, and reactions of these materials are discussed. X-ray crystallographic data on several metallocarboranes is presented. Empirical rules governing rearrangement reactions and stability of metallocarboranes are also presented.