

REVIEWS OF MODERN PHYSICS

VOLUME 32, NUMBER 2

APRIL, 1960

Papers from the Conference on Molecular Quantum Mechanics, Held at the University of Colorado, Boulder, Colorado, June 21-27, 1959

Introductory Note

ROBERT G. PARR

Department of Chemistry, Carnegie Institute of Technology, Pittsburgh 13, Pennsylvania

THE following papers emanate from the Conference on Molecular Quantum Mechanics which was held on the campus of the University of Colorado in June, 1959. Sponsored by the National Science Foundation, this conference was organized by a steering committee consisting of J. O. Hirschfelder (University of Wisconsin), R. S. Mulliken (University of Chicago), R. Pariser (DuPont Company), W. T. Simpson (University of Washington), J. C. Slater (Massachusetts Institute of Technology), J. de Heer (University of Colorado), J. H. McMillen (National Science Foundation), and R. G. Parr, chairman (Carnegie Institute of Technology). More than one hundred scientists attended, eighteen of whom came from abroad.

The titles for the ten conference sessions show its plan and scope: Atoms and Small Molecules I; Atoms and Small Molecules II; Atoms and Small Molecules III; The Many-Body Problem, Density Matrices; Atoms in Molecules Methods, Nature of the Chemical Bond; Reaction Rates, Intermolecular Forces; Complex Molecules; Problems in Structure and Spectra I; NMR-ESR-QR Spectroscopy; Problems in Structure and Spectra II. The papers which follow are arranged in a similar order, except that placed first is the informal

talk given by Professor Coulson after the banquet on the final evening.

The eighth conference session was designated the William E. Moffitt Memorial Session. Coulson presided, and papers were presented by Liehr, Moscovitz, Waserman, Hijikata, and Berry.

We are indebted to Dean Little, Mr. Bartram, and other officials of the University of Colorado for much help. The hospitality proffered the conference participants by everyone at the university is memorable. Special thanks are due Professor de Heer and Professor Simpson, and Professor E. U. Condon.

The approximately forty papers in this collection represent contemporary good work in the field of molecular quantum mechanics, but they should not be regarded as providing a complete review or a balanced picture of this research field. Quite accidentally there are no papers on ligand-field theory, for example, and certain laboratories are inadequately represented. But read as a group these papers should pretty well indicate how this field stands today.

An informal account of the conference, prepared by K. Ruedenberg of Iowa State College, may be found in the May, 1960 issue of *Physics Today*.