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A Program for Preparation of a Modernized Version of Groth's Chemische Kristallographie

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A procedure has been introduced for the recording and storage of data in crystal chemistry and physics, which permits its transfer to IBM BCD magnetic tape in a form most efficient for IBM 704 machine input for a wide variety of crystallographic computations, and for printout by IBM 407 tabulators or cardatype machines, according to any desired categories, and directly onto reproducing (Multilith) mats. Efficient data-abstracting procedures for punched-card primary input, and methods of proof-reading and editing, have been developed. Using these new techniques, a program is in progress to record all crystal data, to compare and evaluate results from various types of measurements, and to carry out automatically all feasible crystallographic computations — including those bearing on morphology, structure analyses and their results, crystal physics, etc.

The program will require about three years for abstracting, recording and treatment of all secondary sources, within the Groth Institute. Abstracting of primary literature will be initiated shortly in this Institute and in various collaborating laboratories throughout the world.

The program is directed by an expanding staff of resident and corresponding editors, organized according to both regional and topical categories. Collaborating scientists will have access to all information of interest to them, treated and classified as desired.

Among the results of these activities will be regularly-published monographs on special crystallographic topics, listings of missing or incomplete or contradictory data, and recommendations for special measurements. Methods for automatization of data gathering, such as for morphological measurements and crystal drawing, and x-ray and neutron diffraction data collection from single crystals, will be provided to collaborators; and, as soon as feasible, some instruments for these purposes will be distributed to key laboratories in various countries. Completed programs for automatic IBM 704 computations will likewise be available. The majority of such automatic 704 programs, the need for which has been envisaged, are already completed and tested.

The mass of crystallographic data which will therewith be provided is so great that it is not feasible to publish all of it. Consequently, the Groth Institute and collaborating central institutions will serve as sources of computed data, as these are requested for limited distribution requirements. Approximately five years hence, information provided by these programs will be used for the inception of writing of a new edition of Paul von Groth's Chemische Krystallographie. Groth's chemical classification scheme will be retained in one section of this encyclopedia; but a second section will incorporate special topics in crystal chemistry and physics, prepared by experts in the respective subjects who will have available to them all of the stored and computed material of the Institute and associated

organizations.

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