Computational Methods for the Determination of Formation Constants (Modern Inorganic Chemistry)

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This volume is concerned with methods that are available for the calculation of for mation constants, in particular computational procedures. Although graphical meth ods have considerable value in the exploration of primary (raw) data they have been overtaken by computational methods, which, for the most part, take primary data and return the refined formation constants. Graphical methods are now considered com plementary to these general computational procedures. This volume brings together programs that span the lifetime of computer-assisted determination of formation constants. On one hand the reader will find listings of programs that are derived from LETAGROP (b.l961) and the GAUSS-G/SCOGS (b. 1962) families. On the other hand programs are presented that are the newest mem bers of the SCOGS lineage and from the on-going MINIQUAD series. One program is presented that describes a computational approach to the classical Hedstrom Osterberg methods; another that takes care of electrode calibration in a simple yet rigorous manner. Potentiometry and spectrophotometry are the most popular experimental tech niques for equilibrium studies, and the programs in this volume reflect this. Four programs handle potentiometric data, two will process spectrophotometric data, and one makes use of both types of data separately or in combination.

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