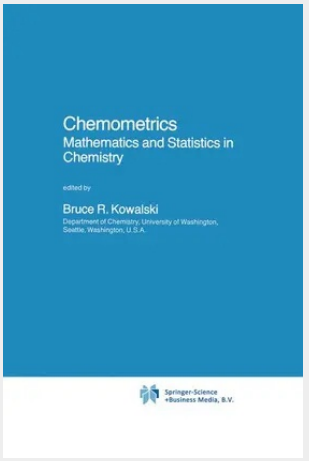
Kowalski

Chemometrics

Mathematics and Statistics in Chemistry



At a time when computerized laboratory automation is producing a da ta explosion, chemists are turning to applied mathematics and statistics for the tools to extract useful chemical information from data. This rush to find applicable methods has lead to a somewhat confusing body of literature that represents a barrier to chemists wishing to learn more about chemometrics. The confusion results partly from the mixing of chemical notation and nomenclature with those of statistics, applied mathematics and engineering. Additionally, in the absence of collaboration with mathematicians, chemists have, at times, misused data analysis methodology and even reinvented methods that have seen years of service in other fields. The Chemometrics Society has worked hard to solve this problem since it was founded in 1974 with the goal of improving communications between the chemical sciences and applied mathe matics and statistics. The NATO Advanced Study Institute on Chemometrics is evidence of this fact as it was initiated in response to a call from its membership for advanced training in several areas of chemometrics. This Institute focused on current theory and application in the new field of Chemometrics: Use of mathematical and statistical methods, Ca) to design or select optimal measurement procedures and experiments; and Cb) to provide maximum chemical information by analyzing chemical data. The Institute had two formal themes and two informal themes.

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