

Applications of Numerical Methods in **MOLECULAR SPECTROSCOPY**



Pelikán • Čeppan • Liška

Applications Of Numerical Methods In Molecular Spectroscopy Fundamental Applied Aspects Of Chemometrics

John M. Chalmers, Peter R. Griffiths



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Applications of Numerical Methods in Molecular Spectroscopy Peter Pelikan, Michal Ceppan, Marek Liska, 1994-01-19 Applications of Numerical Methods in Molecular Spectroscopy provides a mathematical background theoretical perspective and review of spectral data processing methods The book discusses methods of complex spectral profile separation into bands factor analysis methods methods of quantitative analysis in molecular spectroscopy and reflectance spectroscopy and new data processing methods Mathematical methods in special areas of molecular spectroscopy such as color science electron spin resonance and nuclear magnetic resonance spectroscopies are also covered The book will benefit researchers and postgraduate students in fields of chemistry physics and biology

Chemometrics in Spectroscopy Howard Mark, Jerry Workman Jr., 2018-07-13 Chemometrics in Spectroscopy Second Edition provides the reader with the methodology crucial to apply chemometrics to real world data It allows scientists using spectroscopic instruments to find explanations and solutions to their problems when they are confronted with unexpected and unexplained results Unlike other books on these topics it explains the root causes of the phenomena that lead to these results While books on NIR spectroscopy sometimes cover basic chemometrics they do not mention many of the advanced topics this book discusses In addition traditional chemometrics books do not cover spectroscopy to the point of understanding the basis for the underlying phenomena The second edition has been expanded with 50% more content covering advances in the field that have occurred in the last 10 years including calibration transfer units of measure in spectroscopy principal components clinical data reporting classical least squares regression models spectral transfer and more Written in the column format of the authors online magazine Presents topical and important chapters for those involved in analysis work both research and routine Focuses on practical issues in the implementation of chemometrics for NIR Spectroscopy Includes a companion website with 350 additional color figures that illustrate CLS concepts

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