Multiwavelength Analysis of Closed and Open Reactions and of Spectrometric Titrations: VIS-UV-Absorption, CD, ORD, NMR

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Using multiwavelength information for analysis of chemical multicomponent systems a more precise and more significant evaluation can be performed than by analyzing a single progress curve.
First of all the number of linear independent reaction steps of a time dependent reaction system or of a titration system is determined by graphical matrix rank analysis (A-, AD- and ADQ-diagrams) (1-3).
Subsequently, in chemical kinetics a number of new evaluation methods are used for kinetic analysis: In contrast to other methods, absorbance-time curves at different wavelengths are combined for evaluation. Initial concentrations, A_∞-values, molar absorptivities etc. do not need to be known (4).
These methods, which have been developed originally for closed reactions, may be extended to open reactions, too.
Whenever kinetic progress curves cannot be measured directly by spectrophotometric techniques, the methods of multiwavelength analysis may be applied to coupled enzymatic assays, which are specific for single components of the whole reaction system.
In spectrometric titrations, including binding studies, a great number of graphical and numerical methods for evaluation of multiwavelength measurements have been developed during the last years (2,3,5). By means of A-, AD- and ADQ-diagrams the number of (spectroscopically detectable) dissociation equilibria may be determined. Multistep titrations can be separated into their different equilibria. Absolute or relative pK-values may be calculated using linear graphical methods or nonlinear iterative procedures, which combine the whole multiwavelength information.
All methods mentioned above may also be modified for spectrofluorimetric, CD, ORD, NMR measurements etc. (3,5,6).
The advantages of these new methods are demonstrated by several bioorganic reaction systems in the conventional and stopped-flow region and by multistep titrations with up to 4 macroscopic dissociation steps.

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