

Obtaining the Phenomenological Rate Coefficients from Direct Analysis of Experimental Data

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The increase in computer resources together with more sophisticated software makes the direct examination of experimental rate data using master equation methods practical. This approach avoids a number of difficulties and assumptions which are often encountered in analyzing reaction kinetic trace data. This methodology is particularly useful in cases where the decay of the observed species cannot be described by simple exponential or bi-exponential decay curves. A case study for the reaction of OH with ethylene is given and the modifications to the master equation formulation that are needed to do this analysis are discussed.