Infrared spectroscopic investigations of hydroformylation reactions

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The hydroformylation of olefins is an important reaction in industrial organic chemistry. The reaction is applied on a large industrial scale. More than 10^7 t/y of aldehydes are produced via hydroformylation. It is one of the most widely studied reactions in homogeneous catalysis. In order to get detailed mechanistic information on catalytic cycles involved as well as to study degradation processes of catalytic systems analytical methods and its development are of crucial importance. The hydroformylation has intensively stimulated the development of an in situ spectroscopic methodology, especially relying on infrared spectroscopy. A typical and challenging problem of great practical importance in that field is a pure component decomposition of a chemical multicomponent system in which a chemical reaction is monitored by a sequence of infrared spectroscopic measurements. In this paper we present selected aspects of numerical methods which allow to extract from infrared spectroscopic measurements of a multi-component chemical system the spectra of the underlying pure components together with the associated concentration profiles. The methods rely on the class of multivariate curve resolution techniques. These methods are well-established and powerful tools to extract pure component information from spectroscopic data. Unfortunately, these methods suffer from the non-uniqueness of the possible nonnegative factorizations. Usually a continuum of factorizations exists. This fact is well-known under the keyword of rotational ambiguity. The Ansatz which will be presented in this paper is based on the idea to reduce the rotational ambiguity of pure component factorizations by considering only those concentration factors which are possible solutions of the kinetic equations for a properly adapted set of reaction rate constants. The resulting set of reaction rate constants corresponds to those solutions of the rate equations which appear as feasible factors in a pure component factorization. As an application example we discuss spectroscopic investigations on the kinetics of the hydroformylation of 3,3-dimethyl-1-butene with a rhodium monophosphite catalyst.

References: