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DETERMINATION OF KINETIC MODELS BY THE USE OF PATTERN RECOGNITION METHODS

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Thermoanalytical records obtained in homogeneous systems can be interpreted kinetically by the study of information strings, based on the type of concentration dependence of the mechanistic coordinates, shape index and reaction type index (as the signal height or reciprocal halfwidth referred to unit concentration and activation data [1, 2]). These are available experimentally (ca. 3000 DTA and UV plots were studied) and theoretically, using a Gear integration subroutine as a component of an expert system [2].

A prerequisite for the reliable function of this comparing strategy is the existence of a THEOREM OF COMMON KINETIC RUNS, which means that for a definite model such as 'Mechanistic Concentration Code' (= MCC; [3]) does not depend on the activation data or the signal parameters of the steps (proportionality coefficients, as reaction enthalpy for DSC or DTA). Recently it could be revealed that the MCC-strings of all two-step models consist of independent main parts (i.e., first and last element = orders of reference step or the other step, respectively, and 'sign' elements, + or-, between) and parts beside which are partially dependent on signal parameters or, less, activation parameters; however, application of the probability theory confirms [4, 5] that the deviations of individual total strings from the source strings usually do not exceed 10%.

This means reliable kinetic equivalence of different methods and indicates a fundamental pathway to a systematic model search, based on the reaction matrix of the ODE system, which should be probably transferable to heterogeneous kinetics. In this case, the serious problem of the reliability of

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kinetic data, stressed on ICTA 6 in Bratislava by the ICTA Kinetics Committee [6], may be treated from a rather optimistic view.

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