

Editorial

Thermochimica Acta supports and encourages the publication of kinetic results on materials of scientific or technological importance when the work falls within the scope of the journal. Most readers are aware that there exist numerous methods for analyzing thermoanalytical data. These have appeared in print since the development and proliferation of modern thermoanalytical tools such as differential thermal analysis (DTA), differential scanning calorimetry (DSC), and thermogravimetry (TG). These analytical methods are relatively simple to employ and can provide useful kinetic information when appropriately employed. However, care must be exercised in the application of these kinetic methods and the reporting of the results so that true benefit from the kinetic analysis can be obtained.

In order to aid our authors in the preparation of their manuscripts on kinetic analysis of thermoanalytical data, Dr. Andrew Galwey has constructed a set of guidelines for the presentation of kinetic results in this journal. Dr Galwey, a renowned researcher in the field of kinetics and a member of the Editorial Board of Thermochimica Acta, prepared the guidelines at the request of the editors. The guidelines are presented here for use by authors, referees, and the editors. They are printed in the following pages. Authors of kinetics papers should recognize that these guidelines will be applied to their manuscripts during the review process by both the referees and the editors. The guidelines pertain to any regular article, review article, Note, letter to the editor, or papers submitted to special topical issues or conference proceedings.

There are two important features to the guidelines. Firstly, there is a general discussion of what is expected and desired in manuscripts containing kinetic analysis results. Secondly, specific examples are given which illustrate what is not acceptable in an article submitted to Thermochimica Acta.

The editors sincerely hope that the authors will find the guidelines of value in their preparation of manuscripts.

The Editors

Kinetic Papers in Thermochimica Acta
Dr. Andrew Galwey
General (Summary)

Articles concerned with reaction kinetics that will be accepted for publication in TCA are expected to make a significant and identifiable contribution towards advancement of one or more of the following aspects of the subject.

The chemistry (in the widest sense) of the reactions investigated.

The theoretical interpretation of experimentally measured data.

Laboratory techniques used to measure reaction rates.

(Studies must also be concerned with the thermal properties of materials).

Quantitative data should report meaningful estimations of accuracy. Evidence confirming the stoichiometry of the important reactions involved should be provided whenever possible. A justification or explanation for the selection of a particular reaction for study should be given and results discussed in the context of cited references, including work other than the author's own. Reasons for the methods of kinetic analyses selected to interpret measured rate data should be explained. Whenever possible theoretical conclusions should discuss reactivities and mechanisms of the chemical changes studied.

Kinetic Papers in Thermochimica Acta
More detailed comments (positive desiderata)

These are classified below under the headings that are most often used as internal divisions in published articles.

Introduction

Reasons for undertaking the research should explain what aspect of the subject is being advanced by the present report and why this is of interest. Explanations as to why specific compounds were selected for investigation should be given, together with comments on current topical aspects of their chemistry or their advantages as model compounds (when used in development of experimental techniques). Support should be given through references identifying important related studies including work outside the author's own contributions.

Experimental

The experimental technique used must be in accordance with the scope of TCA and should be shown to be relevant to the objectives of the research programme. Where possible more than one experimental method should be used. Some positive justification for the particular method of kinetic analysis used should be given. The conclusions and interpretations must not depend on the particular experimental method.

Stoichiometry

It is desirable to support any kinetic study with confirmatory evidence that characterizes the chemical change occurring. Information concerning the identity and purity of the reactant is important, together with some description of its physical form (crystal, powder, pellet, etc.). It is also necessary to determine the role of changes that precede or accompany reactions (e.g. dehydration, recrystallization, melting, etc.), together with the identification of the participation and significance of any intermediate. The relevant chemical and physical properties of the products should also be characterized and described. Product analyses should confirm that reaction proceeded to completion and that

the constituents of the reactant are fully accounted for in the stoichiometric balance.

Kinetic results

The reliability of kinetic results is substantially increased by a demonstration that behaviour is quantitatively reproducible. Meaningful limits of accuracy (and their justification) should be given for all reported values of quantitatively measured parameters, including rate constants, activation energies and pre-exponential factors, etc. (Errors are much more widely reported in the field of calorimetry.) Units must also be given always. Some discussion of the merits of the chosen method of kinetic analysis should be provided, together with reasons for identifying the reported fit to a given rate equation in preference to possible alternatives.

Rules for reporting rate observations are difficult to formulate in general terms but the graphical presentation of representative yield-time data can be helpful (and should include indications of accuracy or error limits). If calculated values of n , E and A change across the temperature range investigated, this should be reported and explained. Ranges of α , temperature and other parameters across which the studies were completed should be stated. The possible influence of experimental conditions on reported 'compensation effects' should always be critically considered by the author.

The number of significant figures used to report measured parameters and their error ranges must be realistic. Care should be taken to distinguish between statistical scatter and systematic uncertainties.

Discussion

New research observations should be discussed with reference to the widest appropriate field and placed in perspective through references to studies by other workers. Theoretical interpretations of results should include consideration of the significance of calculated parameters, including, for example, the magnitudes of both Arrhenius terms.

Kinetic reports that advance the subject often result from analyses of observations in the context of reliable knowledge of reaction stoichiometry

and with support from information obtained from complementary experimental techniques, for example, microscopy.

Kinetic Papers in Thermochemica Acta More detailed comments (the negative approach)

Introduction

Observations that a particular compound (or group of substances) have ‘not been studied before’ or (worse) ‘are interesting’ (for unspecified reasons) will not be accepted as necessary and sufficient justification for publication.

Experimental

The use of mathematical techniques of analyses of rate data supplied in the computer of an instrument will not be accepted as yielding meaningful kinetic parameters (n , A , E , etc.). Some evidence for

the application of an appropriate method must be given.

Stoichiometry

Reactant identification and purity from the ‘label on the bottle’ should not be sufficient characterization of the reactant. Products guessed at (but not so admitted in the text) should not be reported. Atmosphere influences chemistry in many reaction vessels.

Kinetic results

Print-outs of exact values of kinetic parameters (completed in a computer “black box”) does not constitute an acceptable kinetic result.

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