

Guidelines for Presentation and Analysis of Kinetic Data in Papers

When submitting papers to *Transition Metal Chemistry* which contain kinetic data the authors should follow the guidelines presented below.

- The kinetic data should be analysed by the usual graphical methods. In particular, for the vast majority of reactions which are studied under pseudo first order conditions, the kinetic order for the reagent not in an excess should be determined either by curve-fitting methods or by the appropriate graphical methods. The method used needs to be explained in the Experimental section. The kinetic order for the reagent in an excess should be determined by the usual plots of k_{obs} (or rates) *versus* concentration of reagents. In cases where the rates of reaction depend on the concentrations of several reagents, each of which is varied in individual experiments, each of the corresponding plots should be shown on separate graphs. The lines or curves fitted to the data on these plots should be those defined by the experimental rate law (see below), and this should be referred to in the legend of the figure. Appropriate error bars should be included in the graphs.
- It is usually not appropriate to determine the kinetic orders from plots of $\log(k_{\text{obs}})$ *versus* $\log[\text{reagent}]$, especially if the dependence of k_{obs} on $[\text{reagent}]$ is non-linear (see below). If authors do use such log-log plots they must justify their use in detail in the text and explain why the use of plots of k_{obs} *versus* $[\text{reagent}]$ are inappropriate.
- In cases where the dependence of k_{obs} *versus* $[\text{reagent}]$ is non-linear (*eg* so-called saturation kinetics or inhibition behaviour) the plots should be presented in the text and the curve fitted to the data should be that defined by the experimental rate law (see below). Authors should be aware that in cases where the dependence of k_{obs} *versus* $[\text{reagent}]$ is non-linear, the use of log-log plots is particularly inappropriate since these log-log plots will give a non-integer value for the kinetic order which is meaningless. In reactions exhibiting a non-linear dependence of k_{obs} on the $[\text{reagent}]$ the kinetic order changes with the concentration of the reagent.
- The experimental rate law should be presented in the text as a mathematical equation, with the determined error limits associated with each term. This rate law must accommodate all of the experimental kinetic data. The mathematical form of the experimental rate law should be similar to that of the rate law associated with the proposed mechanism (see below).
- A Scheme presenting the proposed mechanism for the reaction should be presented, together with the derived associated rate law. Chemical structures must be drawn with appropriate software. In general, detailed derivation of rate laws associated with proposed mechanisms need not be included in the main text. The authors should consider including the derivation in supplementary data or as an appendix to the paper. In cases where the derivation is unusual or particularly complicated (especially those involving presumed inequalities), then the derivation should be included in the main text.
- Comparison of the experimental rate law with that associated with the proposed mechanism should include determination of the values of elementary rate and equilibrium constants, and limits to values where limiting forms of rate laws are applicable. The authors should discuss these values in the text, comparing them to analogous values for similar reactions and commenting on the reasonableness of the values.
- Activation parameters (ΔH^\ddagger and ΔS^\ddagger) determined for reactions from measuring the temperature dependence of the reactions need to ensure: (i) that the temperature range covers at least 20°C, or if not to include a justification why a more limited temperature range is used; (ii) that in multistep reactions the individual temperature dependence of each elementary rate and equilibrium constant is determined where possible. In cases where this is not possible the authors should explain to what combination of elementary rate and equilibrium constants the activation parameters correspond.
- Authors should explain in the text how measurement of the effects of ionic strength variation or solvent composition (including dielectric constant variation) adds crucially important mechanistic information to their studies. Where such measurements contribute nothing new to the understanding of the mechanism, such data should not be included.



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