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A Proposal for the Use of a STANDARD FORMAT FOR THE PUBLICATION OF STABILITY CONSTANT MEASUREMENTS

Prepared for publication by

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A proposal for the use of a standard format for the publication of stability constant measurements

INTRODUCTION

This brief statement is submitted on behalf of IUPAC Commission V.6, which is concerned with equilibrium data. Its ongoing projects include the production of critical evaluations of the published stability constants in certain well-defined areas, and a sub-commission is charged with the collection and publication of stability constant data to supplement the volumes already available. In discussing the data, and other information found in the literature, members of the Commission expressed concern at the diversity of ways in which stability constant results are reported, and at the occasional absence of specific information which is critical in the proper evaluation of experimental results, and therefore proposed that a minimum list of requirements be drawn up for the guidance of both authors and editors. An obvious comparison can be made with the field of X-ray crystallography, where there has been considerable success in standardizing the presentation of that information which is judged crucial in the publication of papers on crystal structure.

DISCUSSION

The following points are regarded as important by the Commission and the appropriate information should therefore appear in any paper reporting stability constant measurements.

1. The purity of reagents and solvents, and the procedures followed in solvent or reagent purification.

2. The composition of the solution, especially the ionic strength, and any other relevant factors including the range of metal and ligand concentrations investigated. For mixed solvent systems, the solvent composition must be defined.

3. When appropriate, the pH range over which measurements have been made, the titrant used, and the $\underline{K}_{\omega}$ value assumed.

4. The instrument(s) (e.g. pH meter, electrode, spectrophotometer, etc.) used in the experimental studies, and an explicit description of the method of calibration.

5. The temperature and temperature range.

6. The number of data points recorded in a titration (or elsewhere as appropriate), and the number of replicate measurements.

7. The computer program, or any other method of calculation used to derive final results from the experimental values, and a literature reference if the programs are the work of others; new programs should be shown in terms of the stepwise logic involved. Any discussion of the reasons for choosing a given program may form an appropriate part of the text of the paper.

8. The range of the results, the standard deviation of the final result, the sources of error, and the methods used in establishing these parameters.

The Commission suggests that much of the work on stability constant measurement can be presented in brief tabular form if the points above are followed, and that the publication of long cursive papers whose only purpose is to report quantitative measurements should be discouraged. A sample Table is attached. Special comments can then be placed in the text if the authors, and the editors, find this appropriate.

Finally, it is suggested that some discussion of the reasons which prompted the experiments, and of the chemical information which has subsequently been derived from the measurements, would serve to make stability constant data an intrinsic part of chemistry as a whole, rather than a separate and sometimes esoteric field in itself. Similarly,

TABLE. Summary of Experimental Parameters for the System:

Tyrosyl-glycyl-prolyl-tyrosine/Cu^{II}

Solution Composition	$[T_L]$ range	0.003-0.005 mol dm^{-3}
	$[T_M]$ range	0.001-0.004 mol dm^{-3}
	ionic strength, electrolyte	0.10 mol dm^{-3}, KNO_3
	pH range	protonation: 2.7-10.8
Experimental Method		pH titration, calibrated in concentrations
Temperature		25°C
Total number of data points		protonation: 207; 2 titrations Cu complexation: 274; 3 titrations
Method of Calculation		SUPERQUAD (reference)
Protonation Constants		ligand=H_3L; errors as σ
		$\log \beta_{HL}$=10.16±0.01
		$\log \beta_{H_2L}$=19.96±0.01
		$\log \beta_{H_3L}$=27.50±0.02
		$\log \beta_{H_4L}$=30.52±0.03
Stability Constants		$\log \beta_{CuL}$=10.29±0.09
		$\log \beta_{CuHL}$=19.70±0.01
		$\log \beta_{CuH_2L}$=24.36±0.05
		$\log \beta_{Cu_2L_2}$=24.00±0.05
		$\log \beta_{Cu_2H_2L_2}$=3.66±0.02

comparisons with previous determinations on identical or similar metal ligand systems would help to place new work in context. It appears that far too much stability constant work is concerned with measurements which are made without any aim of extending the chemistry of the metal or the ligand, and such papers do little to strengthen the Commission's conviction that stability constant measurements do indeed give useful quantitative chemical information, and information which can be usefully related to other structural and preparative studies.