# INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

## ANALYTICAL CHEMISTRY DIVISION COMMISSION ON ANALYTICAL NOMENCLATURE

# RECOMMENDED NOMENCLATURE FOR LIQUID\_LIQUID DISTRIBUTION

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## ANALYTICAL CHEMISTRY DIVISION COMMISSION ON ANALYTICAL NOMENCLATURE<sup>†</sup>

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#### INTRODUCTION

The authorship of this report cannot clearly be defined since it has been drafted and redrafted many times. It therefore represents the carefully considered opinions and recommendations of several 'generations' of the Nomenclature Commission of the Analytical Chemistry Division of the IUPAC. The penultimate version was widely circulated in the IUPAC Information Bulletin No. 26 and this final version was drafted by H. M. N. H. Irving for the Commission in the light of all the comments received following the publication and from the Analytical Chemistry Division's inter-commission *ad hoc* working group on the nomenclature of separation processes, where the membership was: D. N. Hume (Chairman), H. G. Helfferich, L. B. Rogers, T. S. West.

### RECOMMENDED TERMINOLOGY OF LIQUID-LIQUID DISTRIBUTION AND EXTRACTION

1. Liquid-liquid distribution. The process of transferring a dissolved substance from one liquid phase to another (immiscible) liquid phase; the corresponding method of separation and concentration.

Comment. A synonymous term for liquid-liquid distribution is partition between two liquids. The terms solvent extraction or liquid extraction are not recommended.

## 2. Liquid-liquid extraction

Comment. This is a special case of liquid-liquid distribution and the term can be used where it is more appropriate.

3. Extraction constant,  $K_{ex}$ . The equilibrium constant of the distribution reaction. At zero ionic strength it is expressed as  $K_{x}^{\circ}$ .

Comment. For example in the gross reaction

 $M_{w}^{n+} + nHL_{org} \Rightarrow ML_{n org} + nH_{w}^{+}$ 

(w = aqueous phase, org = organic phase)

in which the reagent HL initially dissolved in an organic phase reacts with a metal ion in aqueous solution to form a product,  $ML_n$ , which is more

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soluble in the organic phase than in water, the equilibrium constant may be written as

$$K_{\text{ex}} = \frac{[\text{ML}_n]_{\text{org}} [\text{H}^+]_w^n}{[\text{M}^{n+}]_w [\text{HL}]_{\text{org}}^n}$$

The phases can also be specified by the formula of the solvent, or by the subscript o or org (to be defined in the text) or by overlining formulae referring to one phase, usually the less polar phase. The subscript w (or aq) is usually omitted.

When the reagent is more soluble in water than in the other immiscible phase it may be more convenient to define a special extraction constant in terms of  $[HL]_w$ . In distribution equilibria involving only non-aqueous systems (e.g.  $SO_2(l)$ , molten salts and metals) the mass action constant for the relevant process can be identified with  $K_{ex}$ .

4. Distribution constant,  $K_D$ . The ratio of the concentration of a substance in a single definite form in the organic solvent phase to its concentration in the same form in the aqueous phase at equilibrium, frequently termed a partition coefficient.

$$(K_{\mathrm{D}})_{\mathrm{A}} = [\mathrm{A}]_{\mathrm{o}}/[\mathrm{A}]_{\mathrm{w}}$$

*Comment.* The use of the inverse concentration ratio (aqueous/organic) or the ratio of the concentration of the lighter phase to the concentration in the denser phase is not recommended.

5. Partition constant,  $K_{D}^{\circ}$ . The value of  $K_{D}$  at zero ionic strength.

6. (Concentration) Distribution ratio,  $D_{\rm C}$ . The ratio of the total analytical concentration of a substance in the organic phase to its analytical concentration in the aqueous phase, usually at equilibrium. (The descriptive adjective concentration can be omitted when there is no ambiguity with the Mass Distribution Ratio  $D_{\rm m}$ .)

Comment. The term distribution or extraction coefficient can be used in place of distribution ratio. However, the terms partition constant or partition coefficient should not be used in this connection since there has been confusion in the past between its use to describe a distribution ratio which varies with experimental conditions (e.g. pH, presence of complexing agents) and a true partition constant,  $K_{\rm D}^{\circ}$ , which is by definition invariable (cf. paragraph 5) or a distribution constant  $K_{\rm D}$  which is constant for a particular species under specified conditions.

7. Recovery factor, R. The fraction or percentage  $(R_{\%})$  of the total quantity of a substance extracted (usually into the organic solvent phase) under specified conditions.  $R_A = Q_A/(Q_A)_0$ , where  $(Q_A)_0$  and  $Q_A$  are the original and final quantities of the substance A.

Comment. The term extractability is not recommended. If an aqueous solution is extracted with n successive portions of organic solvent, the ratio of the volumes of the phases being  $V_0/V_w = r$  each time, the recovery factor for a particular substance is given by

$$R_n = 1 - (rD_c + 1)^{-n}$$
.

If n = 1 and r = 1,  $R_1 = D_c/(1 + D_c)$ .

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**8. Enrichment factor, S.** The factor by which the original ratio of two substances to be separated must be multiplied to give the ratio after separation (usually in the organic phase).

$$rac{Q_B}{Q_A} = S_B/_A \, rac{(Q_B)_{f o}}{(Q_A)_{f o}}$$

Hence

$$S_B/_A = Q_B(Q_A)_0/Q_A(Q_B)_0 = R_B/R_A$$

Comment. In any analytically useful separation,  $R_A \sim 1$ , so that  $S_B/_A \sim R_B$ . In terms of D, n and r, the enrichment factor is given by

$$S_B/A = \frac{1 - (1 + rD_B)^{-n}}{1 - (1 - rD_A)^{-n}}$$

If n = 1 and r = 1,  $S_B/A = D_B(1 + D_A)/D_A(1 + D_B)$ .

Comment. In liquid-liquid extraction distributions the enrichment factor is not given by  $D_B/D_A$  as often stated.

**9. Extractant.** A liquid phase (usually an organic solvent or the solution of an extracting agent in an organic solvent or solvent mixture) which is used to extract a substance from another liquid phase (usually aqueous).

Comment. This term should not be applied to one of the components of the extracting phase.

10. Diluent. An inert (organic) solvent used to improve the physical properties (density, viscosity, etc.), or the extractive properties (e.g. selectivity) of the extractant.

11. Extracting agent. The reagent which forms a complex salt or other adduct which partitions across the phase boundary of the extraction system. 12. Extract. The separated phase (usually organic) containing the substance extracted from the other phase.

13. Stripping (back-extraction). The process of back-extraction of the substance from the extract (usually into an aqueous phase).

14. Stripping solution. A solution (usually aqueous, sometimes water alone) used for extracting the substance from the extract (usually organic).

15. Scrubbing. The process of removing impurities from the separated phase containing the main substance (i.e. from the extract or *back-extract*).

16. Scrubbing solution. An aqueous or organic solution used for scrubbing.17. Salting out. Improving the extraction of a substance by the addition of an electrolyte to the aqueous phase.

Comment. The term salting-out is used here in a wider sense than it is in some other fields.