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Partition coefficient (1-octanol/water)— Shake flask method

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Foreword

This translation has been made based on the original Japanese Industrial Standard established by the Minister of International Trade and Industry through deliberations at the Japanese Industrial Standards Committee according to the proposal of establishing a Japanese Industrial Standard from Japan Chemical Industry Association (JCIA)/Japanese Standards Association (JSA), with a draft of Industrial Standard based on the provision of Clause 1, Article 12 of the Industrial Standardization Law.

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Partition coefficient (1-octanol/water)— Shake flask method

Introduction This Japanese Industrial Standard has been prepared based on OECD Guideline for the testing of chemicals 107, *Partition coefficient (n-octanol/water) : Shake flask method* without changing the technical contents.

The portions sidelined or underlined with dots and Annex 1 are the matters not stated in the original OECD Guideline for the testing of chemicals.

Remarks : This Standard employs the term “1-octanol” used in the Japanese Industrial Standard instead of “n-octanol” which is used in the original OECD Guideline 107.

1 Scope This Standard specifies shake flask method for the determination of partition coefficient (1-octanol/water), hereafter referred to as “ P_{ow} ”.

P_{ow} values in the range $\log P_{ow}$ between -2 and 4 (occasionally up to 5) can be experimentally determined by the method set out in this Standard [see (1), (2) of Annex A].

The shake flask method is impossible to use with surface-active materials.

2 Normative references The following standards contain provisions which, through reference in this Standard, constitute provisions of this Standard. The most recent editions of the standards (including amendments) indicated below shall apply.

OECD GUIDELINE FOR THE TESTING OF CHEMICALS, No. 105 “Water Solubility” (Adopted by the Council on 27 July, 1995).

OECD GUIDELINE FOR THE TESTING OF CHEMICALS, No. 111 “Hydrolysis as a Function of pH” (Adopted by the Council on 12 May, 1981).

OECD GUIDELINE FOR THE TESTING OF CHEMICALS, No. 112 “Dissociation Constants in Water” (Adopted by the Council on 12 May, 1981).

OECD GUIDELINE FOR THE TESTING OF CHEMICALS, No. 115 “Surface Tension of Aqueous Solutions” (Adopted by the Council on 27 July, 1995).

3 Definitions and units For the purposes of this Standard, the following definitions and units shall apply.

partition coefficient (P), defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of two largely immiscible solvents. In the case of 1-octanol and water:

$$P_{ow} = \frac{C_{1-octanol}}{C_{water}}$$

The partition coefficient, being the quotient of two concentrations, or the quotient of the fractions of the test substance in the two phases multiplied by a fixed volume ratio, is dimensionless and is usually given in the form of its logarithm to base ten.

4 Principle of the method The Nernst partition law applies at constant temperature, pressure and pH for dilute solutions. It strictly applies to a pure substance dispersed between two pure solvents and when the concentration of the solute in either phase is not more than 0.01 mol per litre. If several different solutes occur in one or both phases at the same time, this may affect the results. Dissociation or association of the dissolved molecules result in deviations from the partition law. Such deviations are indicated by the fact that the partition coefficient becomes dependent upon the concentration. Measurements should be made on ionizable substances only in their non-ionized form (free acid or free base) produced by the use of an appropriate buffer with a pH of at least one unit below (free acid) or above (free base) the pK .

5 Preliminary information on the test substance Before carrying out the test, the following information about the test substance shall be known:

- a) structural formula;
- b) water solubility (OECD Guideline for testing chemicals 105);
- c) hydrolysis as a function of pH (OECD Guideline for testing chemicals 111);
- d) dissociation constants in water (OECD Guideline for testing chemicals 112);
- e) 1-octanol solubility;
- f) surface tension of aqueous solutions (OECD Guideline for testing chemicals 115);
- g) analysis method which is higher selective to the test substance.

6 Reference substances Reference substances do not need to be employed. They serve primarily to check the performance of the method from time to time and to allow comparison with results from other methods.

7 Description of the method

7.1 Apparatus and instruments The following apparatus and instruments should be prepared for the measurement.

bottles for mutual saturation, glassware used in clause 7.3 (stock bottles, etc.).

shaker or stirrer, the reciprocating shaker or the magnetic stirrer, which is capable of shaking or stirring quietly.

thermostat, constant-temperature water bath, or thermostatic chamber, capable of maintaining test temperature.

centrifuge, capable of maintaining test temperature in the case where it is attached with the temperature controller.

mechanical shaker When using a mechanical shaker for equilibrium, it is recommended to rotate the vessel through 180 degrees about its transverse axis (20 turns per minute).

vessel for equilibrium, glassware such as centrifuge tube with ground-in stopper, flask, and fluororesin and stainless steels for the material of the vessels are applicable, which do not cause the mutual reaction with the test substance.