Formulation Design with Organic Conception Diagram

1. Introduction

The "Organic Conception Diagram" has been widely applied especially in the field of environmental chemistry, pharmaceutical chemistry, etc. as means that express the property of organic materials that feature relatively complex interactions. Ever since our discover of the fact that the Organic Conception Diagram provides a sure guide for assessment of a surfactant, we have been prescribing and assessing surfactants using the Organic Conception Diagram.

Combining the Organic Conception Diagrams accumulated in our company with the various types of emulsifier prescriptions, we have established the "Formulation Design with Organic Conception Diagram", and efficiently provide customers with a prescription that fills the needs of the customer. We have a small booklet that explains how to make a prescription on the basis of Organic Conception Diagram. If you need more information than this general explanation, please ask us for the booklet. We are also prepared to visit customers to provide lectures, and awaiting your requests. (Regarding the details of "Organic Conception Diagram", please refer to "Qualitative analysis of organic substance: by Makoto Fujita", etc.)

• Material Request
• Formulation Design with Organic Conception Diagram Booklet(PDF/1.83MB)

2. What is an Organic Conception Diagram?

TOP

In any chemical compound, the property depends much on the various types of intermolecular forces between molecules. The intermolecular force consists mainly of Van Der Waals force by the molecular mass and the electric affinity by the polarity of molecules. As the functional group of the chemical compound differs, it affects much on the boiling point, the refractive index, etc. of the compound. If each of the Van Der Waals force and the electric affinity, which affect much on the property of the compound, could be identified individually, the characteristics of a new, unknown compound or a mixture of such compounds would be predictable.

Unfortunately, it is very difficult to individually and directly measure the Van Der Waals force or the electric affinity. It is not exaggerating to state that it is virtually impossible to measure such factors on daily basis and apply to industrial purposes in order to predict the characteristics of a compound. For that reason, in the principles of Organic Conception Diagram, instead of expressing the intermolecular force, that affects much on the property of a chemical compound, in a direct numeric number, the "boiling point of a material", which is easy to measure and to assess, is used as an index to express the nature of a material.

In the compounds of an identical group having identical functional group, the boiling points of the compounds fall on a curve independently drawn for each of the functional group, and exhibit regular variations depending on the difference of carbon numbers. That is, it means that the property of the material in terms of physical chemistry varies depending upon the changes of the molecular weight, i. e., the functional group. Such changes of the property of a compound are seen on other characteristics such as the refractive index, which means "the boiling point of a compound serves as an indicator by which various properties of the compound in terms of physical chemistry can be predicted".

In the principles of Organic Conception Diagram, the property of a compound in terms of physical chemistry is considered in such a way that the property that depends much on Van Der Waals force is called "organic" and the one that depends much on electric affinity is called "inorganic", thus considering the property of a compound as a combination of "organic" and "inorganic" natures.

Especially when considering the factors that affect various characteristics of an organic compound having hydrocarbons in its basic structure, it can be considered that the characteristics are based on two factors, i.e., the "organic nature" of hydrocarbons composed of the chain of covalent bonds of carbon chains and the "inorganic nature" from the influence of the electric affinity (ion) that exists in the substitution radicals (functional group).

Accordingly, one can easily imagine that the characteristics of an organic chemical compound can be predicted by identifying the characteristic values of the "organic nature" and the "inorganic nature" that are inherent to each compound. That is, the identification of general trends of the "organic nature" and the "inorganic nature", on which the principles of Organic Conception Diagram is based, by accumulating data taken from facts such as the boiling point, the dipole efficiency, etc. allows prediction of the characteristics of a compound or a mixture of compounds.

When the data from a large number of chemical compounds are marked on the Organic Conception Diagram, various trends specific to that property are found in each region of the Organic Conception Diagram. Conversely, it could mean that if the organic value and the inorganic value of an unknown

compound were determined from the structural formula or other factors, the characteristics of the compound could be predicted.

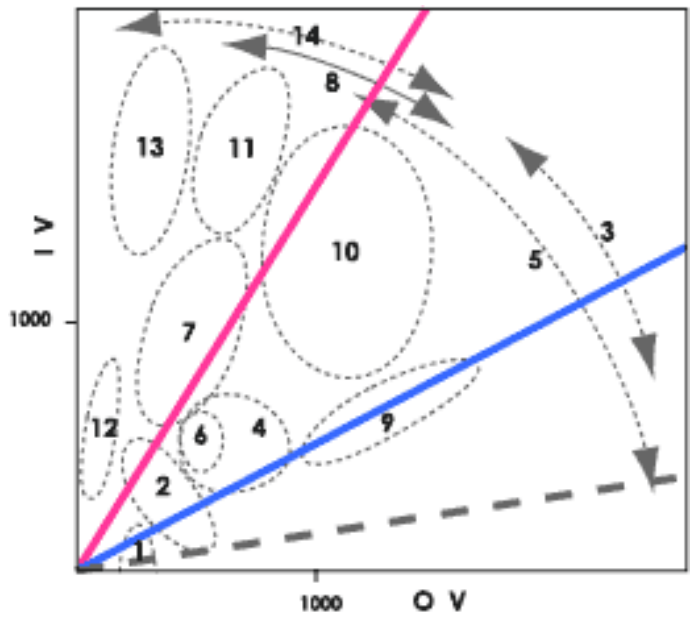

Figure 1. Concept diagram of similar chemical compounds

No.	α	Usage	No.	α	Usage
1	0° ~ 40°	Oil-soluble solution	8	55° ~ 75°	O/W-SAA(HLB 8~18)
2	10° ~ 75°	Plasticizer	9	25° ~ 35°	Oil-soluble dye, disperse dye
3	23° ~ 45°	W/O-SAA(HLB 3~6)	10	35° ~ 65°	Organic pigment
4	25° ~ 55°	Cationic SAA	11	65° ~ 75°	Alcohol-soluble dye
5	10° ~ 60°	Non-ionic SAA	12	75° ~ 85°	Alcohol-soluble dye
6	40° ~ 55°	Foaming intensifier	13	75° ~ 85°	Water-soluble dye
7	55° ~ 75°	Anionic SAA detergent	14	55° ~ 85°	Water-soluble high polymer (protective colloid)

"Organic value" or "inorganic value" is determined as a sum of values from each structural component of the compound.

Table 1.
Organic radicals, organic cum organic/inorganic radicals (subtract)

Inorganic radical	inorganic value	Organic cum organic /inorganic radical	Organic	Inorganic
Light metal	500<	R4Bi-OH	80	250
Heavy metal, amine and NH4 salt	400<	R4Sb-OH	60	250
-AsO3H2,>AsO2H	300	R4As-CH	40	250
-SO2-NH-CO-,-N=N-NH2	260	R4P-OH	20	250
-->N^+-OH,-SO3H,-NHSO2-NH	250	-O-SO3H	20	220
-CO-NHCO-NHCO-	250	>SO2	40	170
≡S-OH,-CONH-CONH-CONH-, -SO2NH-	240	>SO	40	140
Double bond	3	-Cl	40	10
Triple bond	2	-F	5	5
-(OCH2CH2)-,Under cloud point	75	iso-branch	-10	0
-(OCH2CH2)-,Above cloud point	20	tert-branch	-20	0

3. Organic Conception Diagram principle and HLB method

TOP

One of the methods generally used for evaluation of a surfactant is the HLB (Hydrophile Lipophile Balance) method. In that method, assuming a compound, which is of the most hydrophilic nature with an infinite extension of hydrophilic radicals attached to the lipophilic radicals, in an ethylene-oxide-added type nonionic base surfactant, and regarding the HLB value for that compound as 20, and also regarding the HLB value for a compound of absolutely no lipophilic nature as 0, the HLB value of a compound is determined as a relative value compared to the above mentioned values. That is, an HLB value can be considered as an indicator of the balance between the lipophilic nature and the hydrophilic nature. Now, as you compare the HLB method to the Organic Conception Diagram principle, you may realize that the lipophilic nature in an HLB value corresponds to the concept of inorganic nature in the Organic Conception Diagram principle, and the hydrophilic nature matches with the concept of organic nature. As the ratio of an organic value and an inorganic value in the Organic Conception Diagram principle is provided by "inorganic value (IV)/organic value (OV) = IOB", when the IOB value and the HLB value of a compound is compared, the following relationship can be established as an approximate equation.

HLB value = IOB value x 10

Now, as we understand that an HLB value can be converted to an IOB value of the Organic Conception Diagram principle, let's think about how the HLB value is indicated on the Organic Conception Diagram. Supposing the angle included in the organic axis and the line drawn from the origin of the coordinates to the point that a compound occupies as α, as there is such a relationship as

"tanα = inorganic value/organic value", if the points located for compounds having the same IOB value are connected one after another, it will make a straight line that passes the origin with an angleα. That is, the place where the compound having a certain HLB value is located on the Organic Conception Diagram also forms a straight line that passes through the origin, which indicates the relationship between the Organic Conception Diagram and the HLB method. In the Organic Conception Diagram principle, that straight line is called "HLB line", which is shown below.

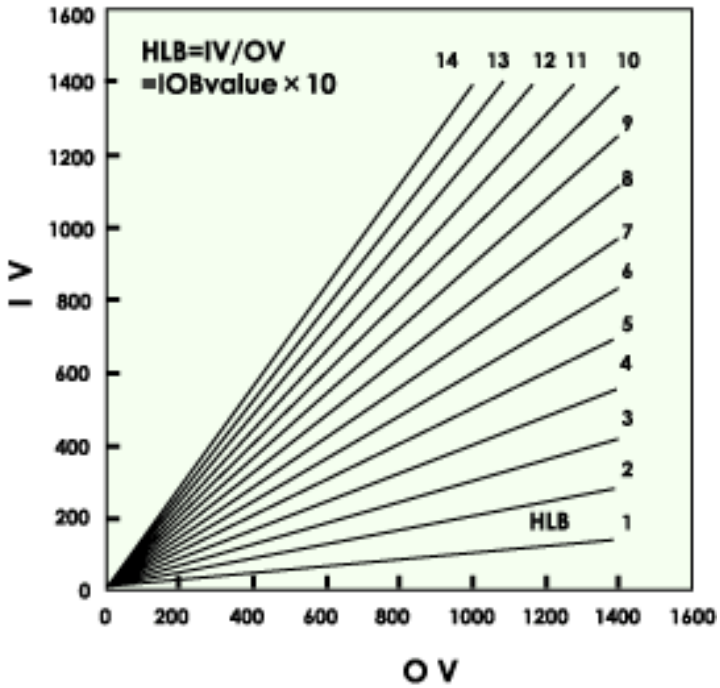

Figure 2. HLB by Oda system and concept diagram

4. rescription by Organic Conception Diagram

TOP

While the HLB value is generally used in prescribing an emulsifier, we have been applying "prescription by Organic Conception Diagram" from the past. As known, the characteristics of the hydrophilic compound, the lipophilic compound and the surfactant affect delicately with each other when prescribing an emulsifier. Since the HLB value method indicates the property of the compound only by the HLB value, it is relatively difficult to accurately indicate the property of various kinds of compounds and accurately identify the characteristics of a mixture of such compounds.

In the Organic Conception Diagram, however, by indicating a compound on a plane, even for a mixture of several kinds of compounds, the characteristics of the mixture can be accurately predictable from the position of the spot that each compound occupies (absolute position, relative distance, relative position, etc.) in the plane. When using the Organic Conception Diagram in making a prescription for emulsifying, as you plot the position of each and all of the compounds on an Organic Conception Diagram, various characteristics of the compounds become recognizable. Also, the relationship between the mixing rate in the prescription and the characteristics of the product becomes clearly understandable, thus allowing efficient prediction of all types of emulsifying and their emulsion characteristics such as the type of emulsifying, the sense of lipophile ~ hydrophile, the dispersing in oil or water, the emulsified/solublized conditions, the foaming/defoaming property, viscosity, the temperature stability, the actual oil phase of generated emulsion, the water phase components, etc.

The above mentioned theory means that by choosing in advance the component substances from our

unique "quality/quantity trend table" that fit the requirements of the target emulsion, a consistent prescription can be attained efficiently.
Also, an example is that when a prescription is plotted on the Organic Conception Diagram as shown below, the characteristics indicated in "features of this type" are predictable from our unique tables and diagrams.

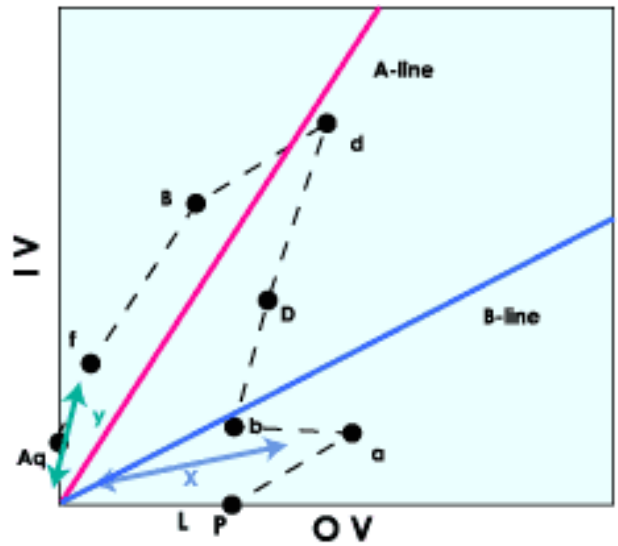

Figure 3. Example of prescription on Organic Conception Diagram

< Features of prescription on Organic Conception Diagram >

(a) An emulsifier having the longest distance from the origin is found near the line A.

(b) The distance (x) from the origin of the water-phase side surfactant having the minimum α value among the oil-phase components is longer than the distance (y) of the water-phase side surfactant having the maximum α value among the water-phase components.

< Features of this type >

(a) This type A is highly hydrophilic, disperses well in water and has a foaming property. When using in a face-cleansing agent, shampoo, etc., slightly emollient characteristics are added (face-cleansing agent, pearl shampoo, lotion)

(b) This type B is most commonly used as a cosmetic foundation material, and enhances the temperature stability. It also has such a feature that it does not whiten after application. (Fundamental cosmetics such as milk lotion, cream, etc.)

5. Closing

TOP

This concludes explanations on the Organic Conception Diagram and the prescription based on it. If you are interested in our unique technique of "emulsifier prescription on the basis of Organic Conception Diagram", please contact to us as we mentioned at the beginning of this article.