THE EFFECTIVE FORMULATION DEVELOPMENT USING THE "ORGANIC CONCEPTUAL DIAGRAM"

(IOB SYSTEM)

Nihon Emulsion Co.,Ltd.

1 For More Effective Development of Formulas

Introduction

Dealing promptly with user needs is the aim in all industries today. Needless to say, effective study of formula has also become an important issue in the cosmetics industry in recent years.Under such circumstances, our company has conceived "The emulsion formula design method using the organic conceptual diagram" as was detailed in this pamphlet in 1950, shortly after the foundation of the firm, and we developed a number of raw materials for cosmetics and emulsion formulas.

The formula designing method includes the prediction of emulsion properties (opacity, state of solubilization, viscosity, lipophilicity/hydrophily, water repellency, dispersion into water, antifoaming/foaming quality) in addition to information on temperature stability and the method of its correction. If they were skillfully utilized, it would be possible to effectively develop intended formulas with minimal emulsification tests. This pamphlet gives an outline of "the design of emulsification formulas using the organic conceptual diagram" unique to our company. We would be happy if your perusal of the pamphlet was to prove useful to your formula researchers.

For More Effective Development of Formulas

2 Organic Conceptual Diagram

IOB SYSTEM Formulation by the organic conceptual diagram based on our company's original idea has been generally known as IOB SYSTEM (inorganic organic balance), and its usefulness highly evaluated as a method of designing formulas and of evaluating properties of materials in the field of cosmetics and other sectors of industries. This pamphlet briefly introduces the IOB SYSTEM. The details are given in another commentary booklet, so you are invited to request the booklet to us.

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2.1 Organic Conceptual Diagram

The "design of emulsion formulas using the organic conceptual diagram", having been practiced in-house, has made it easy to visually determine the physical properties of emulsion by obtaining the two values of "organic value" and "inorganic value" from the chemical constitution of organic compounds, and expressing each ingredient contained in each formulas as a point on a two-dimensional plane called the organic conceptual diagram (Fig.1). It could be easily determined if the organic value was taken to indicate the extent of the lipophilicity (non-polarity) and the inorganic value the intensity of the hydrophily (polarity). According to this method, each ingredient contained in an emulsion formula is expressed on a plane of the organic conceptual diagram, enabling a variety of predictions on the properties of a formula from the positions of each ingredient and the relationship with their quantities.

The specific methods of predicting properties of actual emulsion formula are described in Chapter 3 and following chapters. Explanation is given first on the fundamentals of the organic conceptual diagram.

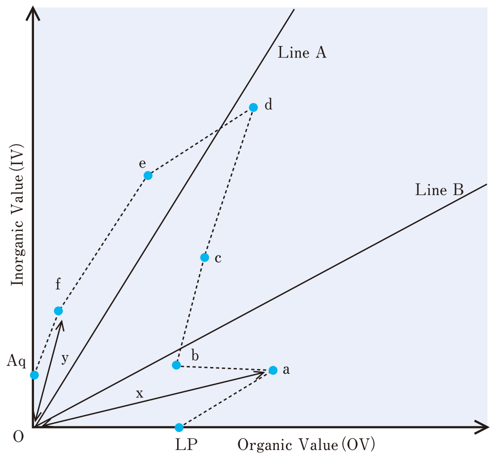


Fig.1 - A formula on the organic conceptual diagram

What are organic value and inorganic value?

2.2 Organic Value and Inorganic Value

In the organic conceptual diagram, a compound is expressed by a combination of two characteristic values, organic value = OV and inorganic value = IV. The organic and inorganic values of a compound are obtained by adding up values predetermined by the groups of compounds (regions)(Table 1) with the whole of respective molecules. An example of calculation is shown in Fig.2. For the details of obtaining the values, please refer to our pamphlet, "Design of emulsion formulas using the organic conceptual diagram". Furthermore, why not use organic values and inorganic values of approximately 3,000 different kinds of raw materials listed in "The collected raw materials for the organic conceptual diagram" of our company, without making calculation every time when it is required.

Table 1 - Organic values and inorganic values

Inorganic radicals	Values	Organic and inorganic radicals	Values	
	Inorganic		Organic	Inorganic
Light metal	500<	R_4P-OH	20	250
Heavy metal, amine and NH_4 salt	400<	$-O-SO_3H$	20	220
$-SO_2-NH-CO-$、$-N=N-NH_2$	260	$>SO_2$	40	170
		Double bond	2	0

Interrelationship with HLB Method

2.3 Organic Conceptual Diagram and HLB

HLB (hydrophile-lipophile balance) generally used to express the surfactant properties, expresses the relative intensity of the properties of hydrophillic and lipophillic groups of surfactants. In the HLB method, the properties of raw materials are expressed by the relative sizes of the HLB values. However, when a formula contains more than several kinds of compounds, it is difficult to predict the properties of the formula by the relative size of the HLB values. In the organic conceptual diagram, not only surfactants, but also all compounds can be deployed and expressed on the two-dimensional organic conceptual diagram so that with respect to mixtures made up of several raw materials, the properties of mixtures to be produced can be predicted more accurately. Moreover, the concept of organic value and inorganic value in the organic conceptual diagram is highly interrelated with the concept of hydrophily and lipophilicity in the HLB method. Therefore, the values obtained from the ratio of organic value to inorganic value as shown in Formula 1 can be used as the HLB value.

POE (10) Monostearate (EMALEX 810)

$C_{17}H_{35}CO \cdot OCH_2CH_2\ (OCH_2CH_2)_{10-1}-OH$

60 75

Organic value = C38×20=760

Inorganic value = 60 (-COOR) +75×9+100 (−OH) =835

(Ester bond for the 1st 1mol in higher fatty acid)

HLB = 10×IOB · · · Formula 1

IOB = Inorganic value/Organic value

(IOB : Inorganic Organic Balance)

Fig.2 - Example of calculation method

2.4 Characteristics Seen in the Organic Conceptual Diagram

The typical properties which can be determined from the positions of each compound plotted on the organic conceptual diagram are shown in Table 2. It can be seen that the organic conceptual diagram is capable of expressing many of the properties necessary for the study of emulsion formulas in a form well arranged. In addition to the properties shown in Table 2, various other properties can be read from the organic conceptual diagram. Fig.3 and Fig.4 shows some of the examples:

Table 2 - Properties that can be read from the organic conceptual diagram

Hydrophily Lipophilicity	Compounds closer to the vertical axis (inorganic axis) have greater hydrophily. Compounds closer to the horizontal axis (organic axis) have greater lipophilicity.
Molecular weight	Molecular weight of compounds of the same series is greater the further the distance from the origin.
Solubility	Compounds on the same ratio line are highly soluble, but become difficult to dissolve as the lines diverge.
Properties	Compounds located close to each other have similar properties.

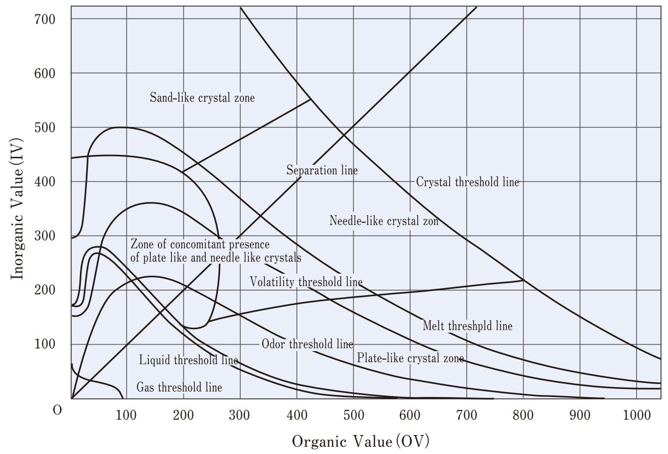
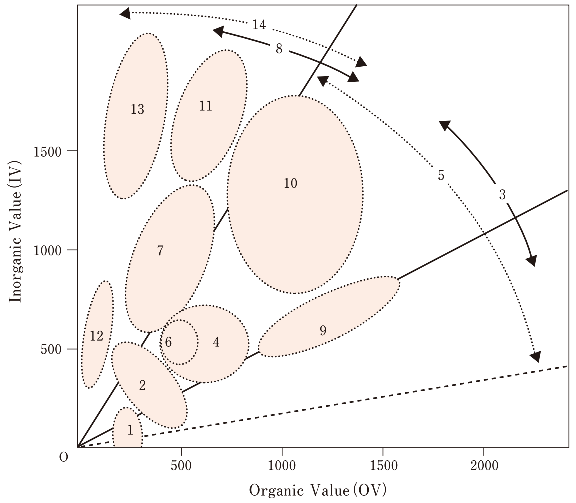


Fig.3 - Characteristics seen in the organic conceptual diagram



No	α (Approx.)	Surfactant	No.	α (Approx.)	Dye stuff, etc.
1	0° ～40°	Oil-soluble solvents	9	25° ～35°	Oil-soluble dyes, dispersion dyes
2	10° ～75°	Plasticizers	10	35° ～65°	Organic pigments
3	23° ～45°	W/O-SAA (HLB 3～6)	11	65° ～75°	Alcohol-soluble dyes
4	25° ～55°	Cation SAA	12	75° ～85°	Introfier, emollient NMF
5	10° ～60°	Nonion SAA	13	75° ～85°	Water-soluble dyes
6	40° ～55°	Foaming auxiliary agents	14	55° ～85°	Water-soluble polymers (protective colloids)
7	55° ～75°	Anion SAA, rinse agents			
8	55° ～75°	O/W-SAA (HLB 8～18)			

Fig.4 - Similar compounds appearing on the organic conceptual diagram

3 Emulsion Formulas and the Organic Conceptual Diagram

3.1 Fields of Use of the Organic Conceptual Diagram

In the organic conceptual diagram, emulsion formulas can be interpreted as a system consist of many ingredients such as oil, surfactant and water. The fields of use of the organic conceptual diagram in the study of emulsion formulas diversify greatly, so all cannot be introduced in this pamphlet. However, we will explain the "prediction of properties of established formulas", "development of new formulas" and "improvement of established formulas", which are the most typical applications. For further details contained in the pamphlet, you are refer to one of our pamphlet "Formulation design by the organic conceptual diagram".

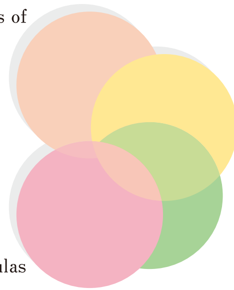


Fig.5 - Applications

3.2 Definitions of Special Terms

Since a number of words with specific meanings are used in the "design of emulsion formulas using the organic conceptual diagram", definitions of such words are given in Table 4. A little care is needed, as some usage is different from general use. In this method of design, in particular, the word "surfactant" denotes all ingredients other than oil having the smallest polarity (α small) in the formula and Aq with the largest polarity (α=90°), irrespective of the properties of actual ingredients.

Table 4 - Explanation of special terms

Long	Distance from the origin of a specific ingredient is long on the organic conception diagram.
Short	Distance from the origin of a specific ingredient is short on the organic conception diagram.
Same ratio line	Lines with constant polar coordinate, α
Type A	Emulsion having much surfactant in the vicinity of Line A
Type B	Emulsion having much surfactant in the vicinity of Line B
ℓA (long A)	Surfactant with the longest distance from the origin is located in the vicinity of Line A among mixed ingredients.
ℓB (long B)	Surfactant with the longest distance from the origin is located in the vicinity of Line B among mixed ingredients.
O	Oil phase (Oil+O_{SAA})
W	Water phase (W_{SAA}+Aq)
SAA	Surfactant
O_{SAA}	Oil phase surfactant
W_{SAA}	Water phase surfactant

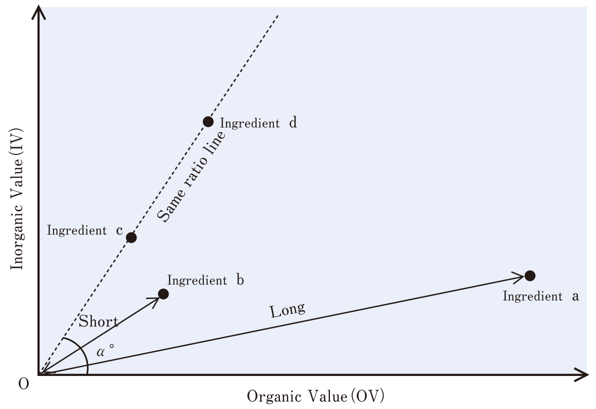


Fig.6 - The Organic conceptual diagram and special terms

Prediction of Properties of Established Formulas

3.3 Prediction of Properties of Established Formulas

The design of emulsion formula using the organic conceptual diagram indicates the type of formula established and enables prediction of the properties, the feel of use from the visual rearrangement of positions of the ingredients plotted on the organic conceptual diagram, and the tendency of the mixed quantities, in accordance with the procedures described below: The prediction of properties is made by first arranging "types of formulas", "tendency of the quantities of ingredients", "tendency of the quantity of surfactant" and "tendency of physical properties of surfactant" then by applying the findings to the "Tendency list of quality and quantity".

Procedure 1 Plotting of Ingredients

Organic and inorganic values of ingredients are determined and plotted on the organic conception diagram. Use the organic and inorganic values given in our pamphlet "collected ingredients for the organic conceptual diagram".

Procedure 2 Entry of Trisection Lines (Line A and Line B)

To determine the balance of surfactant visually easily, enter two lines which divide the angle formed by the axis of least α material among ingredients and inorganic axis, into three equal parts. These two lines are called Line A and Line B. (Fig.7)

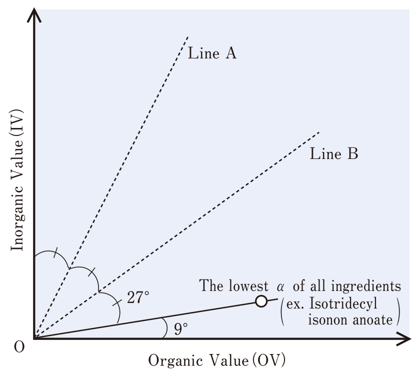


Fig.7 - Trisection Lines

Classification of Formulas

Procedure 3 Classification of the Types of Formulas by Quantity of Ingredients

The types of emulsion are classified by where the the most mixed quantity of surfactant is located on the organic conceptual diagram and how the mixed quantity is distributed.

Type A

Emulsion in which most surfactant is located in the vicinity of Line A and the mixed quantity of surfactant increases toward the vicinity of Line A
(Fig.8):Many Type A are found among emulsion that is washed away, like shampoo.

Type B

Emulsion in which much surfactant is located in the vicinity of Line B and the mixed quantity of surfactant increases toward the vicinity of Line B
(Fig.9):Many Type B are found among coating products like cream.

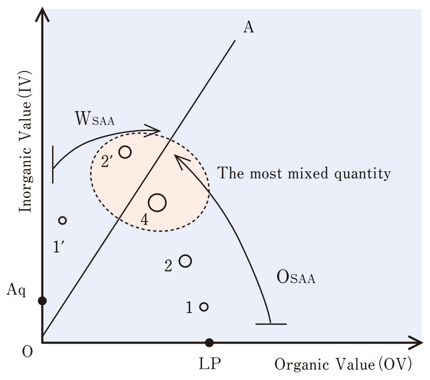


Fig.8 - Tendency of distribution of SAA (Type A)

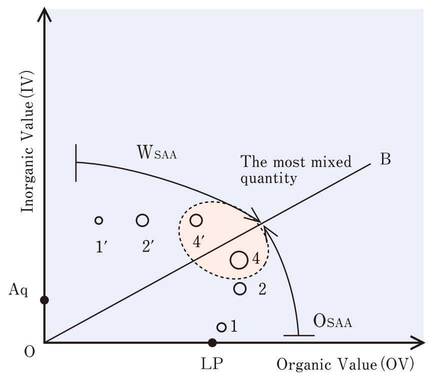


Fig.9 - Tendency of distribution of SAA (Type B)

(Type AC) …Rare case

Emulsion in which the mixed quantity of surfactant increases toward the organic axis and inorganic axis from the vicinity of Line A. (Fig.10)

(Type BC) …Rare case

Emulsion in which the mixed quantity of surfactant increases toward the organic axis and inorganic axis from the vicinity of Line B.(Fig.11)

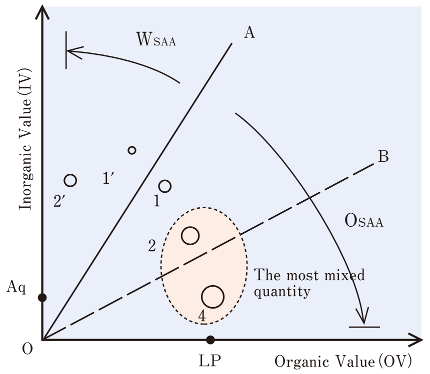


Fig.10 - Tendency of distribution of SAA (Type AC≒Type B)

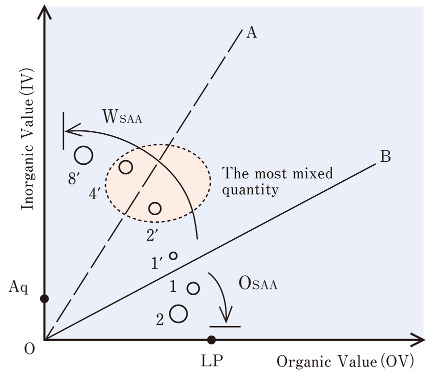


Fig.11 - Tendency of distribution of SAA (Type BC≒Type A)

Procedure 4 Classification of Mixed Ingredients

Defined, by the the types of emulsion described in procedure 3 above, the ratio of quantity of oil phase : quantity of water phase (Quantity of O:W) and the ratio of quantity of surfactant on oil phase : the quantity of surfactant on water phase (O_{SAA}:W_{SAA}) in wt% as shown below:

Type A

In case of Type A formula with most surfactant in the vicinity of Line A, all ingredients existing in the area between the surfactant with low α value to oil, having the lowest α value in all ingredients, is taken as oil phase surfactant (O_{SAA}), and the ingredients existing in the area beyond the Line A and before the inorganic axis (Aq.) is taken as water phase surfactant (W_{SAA}). (Fig.8)

O phase = Oil＋O_{SAA}(0°～Line A)
W phase = W_{SAA}(Line A～<90°)＋Aq

Type B

In the same manner as Type A formula, ingredients existing from that having the next lowest α value to the smallest α value to the Line B are taken as (O_{SAA}), and the ingredients existing in the area beyond Line B and before the inorganic axis (Aq.) are taken as (W_{SAA}). (Fig.9)

O phase = Oil＋O_{SAA} (0°～Line B)
W phase = W_{SAA} (Line B～<90°)＋Aq

Procedure 5 Classification by Positions of Ingredients

(i) ℓA, ℓB

Classification by positions of ingredients is defined by the position of surfactant whose distance from the origin is the furthest. If the SAA located the furthest from the origin in the formula is positioned in the vicinity of Line A, it is classified as ℓA (Fig.12) while if positioned in the vicinity of Line B is classified as: ℓB (Fig.13). (Generally, emulsion having its surfactant with longest distance in the vicinity of either Line A or Line B will tend to be stable.)

(ii) 𝓈 : ℓ, ℓ : 𝓈

For ingredients closest to the inorganic axis or organic axis of the oil phase surfactant (OSAA) or of the water phase surfactant (WSAA), compare their distance from their respective origins to classify "𝓈 : ℓ" and "ℓ : 𝓈". When the distance from the origin of OSAA with the smallest α was taken as x and the distance from the origin of WSAA with the largest α as y and if

$x > y$ it is classified as ℓ : 𝓈 (Fig.12), and if

$x < y$ it is classified as 𝓈 : ℓ (Fig.13)

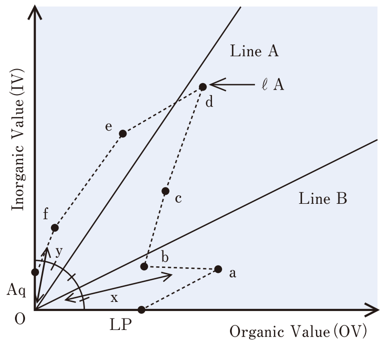


Fig.12 ℓA ℓ : 𝓈

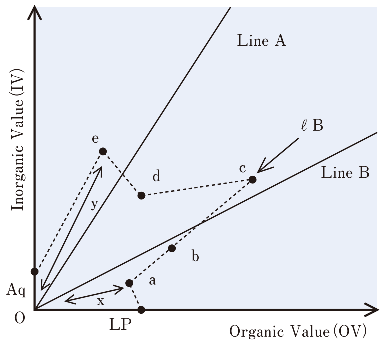


Fig.13 ℓB 𝓈 : ℓ

Prediction of Properties and Feel of Use of Formulas

Procedure 6 Prediction of Properties and Feel of Use

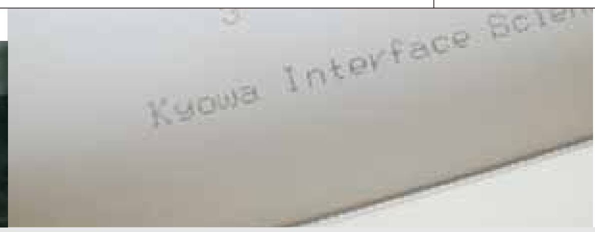
In the foregoing, the types of formulas and mixed ingredients were classified in the procedures 3 to 5. In the design of emulsion formulas using the organic conceptual diagram, the properties of emulsion, temperature stability and the feel of use are predicted by the above mentioned classifications. The prediction of the feel of use is determined from the "type of emulsion" and "classification by positions of ingredients" while that of temperature stability and properties are determined from the "type of emulsion", "classification by positions of ingredients" and "classification and quantities of mixed ingredients", and in reference to our pamphlet "tendency list of quality and quantity".

(i) Prediction of the Feel of Use

The prediction of the feel of use is determined by the combination of the classification of the types of emulsion (Type A or Type B), the classification by position of ingredients (ℓA or ℓB, 𝓈 : ℓ or ℓ : 𝓈) and in reference to the following table: Generally, emulsion formulas can be classified as one of the following:

Table 5 - Types of emulsion formulas and their characteristics

A	ℓA	ℓ : 𝓈	Having a strong hydrophilly being of ℓA, disperses well in water and foaming power is high.	Facial washes, shampoo, skin lotion
		𝓈 : ℓ	Having the strongest hydrophilly and foaming power of all types, because of 𝓈 : ℓ degreasing power is strong to cause the feel of taut and grating	Washing detergent, shampoo
	ℓB	ℓ : 𝓈	The weakest in hydrophily, dispersion in water and foaming power. Generally, with a high viscosity, emollient quality is the strongest among the cleaning agents like facial wash and shampoo.	Facial washes, shampoo, skin lotion
		𝓈 : ℓ	Excellent in hydrophily and foaming power than TypeA, ℓB, ℓ : 𝓈 types. Used most frequently for cleaning agents like shampoo and facial wash.	Rinse shampoo
B	ℓA	ℓ : 𝓈	Used most frequently as a basic cosmetic. Being of ℓA, temperature stability is good. Will not whiten when applied as it is of ℓ : 𝓈.	Milky lotion, cream
		𝓈 : ℓ	Widely used as a basic cosmetic. Temperature stability is the best. Being 𝓈 : ℓ, absorption into the skin is good and fresh. Whitens when applied.	Basic cosmetic with the light feeling
	ℓB	ℓ : 𝓈	A type most strong in the feel of oiliness and water repellency	"Sun care" products, W/O emulsion
		𝓈 : ℓ	Temperature stability is better than TypeB, ℓB, ℓ : 𝓈 type. Though in the feel of use the feel of oiliness is less, water repellency is strong.	"Sun care" products, W/O emulsion



Tendency List of Quality and Quantity

It is necessary for the efficient development of formulas to establish rules for setting parameters for ingredients and its quantity. A vast number of experiments would have to be conducted to obtain the intended emulsion from experiments without rules. Our company therefore conducted emulsification tests by giving a variety of parameters to typical formulas consisting of mineral oil, nonionic surfactants and water, and the results obtained were compiled into the "tendency list of quality and quantity". It has been shown that the list is in high agreement with the general properties of formulas and tendencies despite the evaluation of limited formulas.

(ii) Prediction of Properties

The prediction of properties is made by adding the parameter of quantity to each classification of formula (Type A or Type B, ℓA or ℓB, 𝓈 : ℓ or ℓ : 𝓈) and reading off from the "tendency list of quality and quantity" (Table 6). As for the parameter of quantity, in the list, use O : W, OSAA : WSAA (WSAA/OSAA) and read off the properties in column in which the combination of respective values are closest to the formula. From the "tendency list of quality and quantity", one can read off the tendency of temperature stability of the formula, viscosity, properties and the tendency of dilution in oil or water. An extract of the list and contents, which can be read from each item, is shown here(Table 6). Also, the whole of the tendency list of quality and quantity can be found at the end of the pamphlet.

Table 6 - Tendency list of quality and quantity (Extract)

(日) Phase quantity	(月) Formula No.	Type of emulsion	(火) Selection tendency of surfactant		(水) Temperature stability tendency of formula	(木) Tendency of temperature stability and length LineB~A (Nonion)	(金) O : W 85 : 15 (OSAA : WSAA)	(金) O : W 80 : 20 (OSAA : WSAA)	(祝) Dilution tendency Rp SAA Oil	Rp SAA Aq	SAA increase in quantity Oil	SAA increase in quantity Aq
O>W	1	A	ℓA	ℓ : 𝓈 𝓈 : ℓ	↗	ℓ ↙ ℓ ↙	8.5 : 0.8 (0.1) (土)	8.0 : 0.1 (0.1)	E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↗	𝓈 ↙ 𝓈 ↙						
		B	ℓA	ℓ : 𝓈 𝓈 : ℓ	↙	ℓ ↗ ℓ ↗			E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↙	𝓈 ↗ 𝓈 ↗	(祭) 3 5					
	2	A	ℓA	ℓ : 𝓈 𝓈 : ℓ	↗	ℓ ↙ ℓ ↙	8.5 : 7.1 (0.8)	8.0 : 6.3 (0.8)	E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↗	𝓈 ↙ 𝓈 ↙						
		B	ℓA	ℓ : 𝓈 𝓈 : ℓ	↙	ℓ ↗ ℓ ↗			S	/	S	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↙	𝓈 ↗ 𝓈 ↗	14 12					
	3	A	ℓA	ℓ : 𝓈 𝓈 : ℓ	↗	ℓ ↙ ℓ ↙	7.1 : 8.5 (1.2)	6.3 : 8.0 (1.3)	E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↗	𝓈 ↙ 𝓈 ↙						
		B	ℓA	ℓ : 𝓈 𝓈 : ℓ	↙	ℓ ↗ ℓ ↗	12 15		S	/	S	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↙	𝓈 ↗ 𝓈 ↗						
	4	A	ℓA	ℓ : 𝓈 𝓈 : ℓ	↗	ℓ ↙ ℓ ↙	0.8 : 8.5 (10.6)	1.0 : 8.0 (8.0)	E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↗	𝓈 ↙ 𝓈 ↙						
		B	ℓA	ℓ : 𝓈 𝓈 : ℓ	↙	ℓ ↗ ℓ ↗	5		E	/	E	E
			ℓB	ℓ : 𝓈 𝓈 : ℓ	↙	𝓈 ↗ 𝓈 ↗	10					

①Formula No.

The formula number indicates the classification of a formula by the quantity ratio of O:W, OSAA : WSAA. Formula Nos. 1, 4, 6 and 7 with large difference in the quantity of OSAA : WSAA show the tendency of emulsification, for the formula to emulsify, while the formula Nos. 2, 3, 5 and 8 with little difference in the quantity of OSAA : WSAA show the tendency of semi-solubilization to become bluish emulsion. (In oil of similar distance from the origin, generally, the larger the α the easier the solubilization and the greater the distance of the emulsifier the higher the efficiency of solubilization.)

②Type of emulsion

Classification by the position of ingredients, where the majority of mixed quantity of emulsifier is located (Chapter 3.3.③).

③Selection tendency of Emulsifier

Classification by positions of mixed emulsifiers on the organic conceptual diagram. (Chapter 3.3.④).

④Tendency of temperature stability of formulas

The classifications of ①~③ indicate the general tendency of the temperature stability of formulas. ↗ shows the tendency for stability at high temperatures while ↙ shows the tendency for stability at low temperatures.

Example: Emulsifier of O : W (85:15 ~ 70:30) No.1, TypeA, ℓA tends to be stable at high temperatures.

⑤Temperature stability and tendency of length

It shows the tendency for temperature stability when the length of emulsifiers changes in the range from Line A to Line B.

Example: The emulsifier of O : W (85 : 15 ~ 70 : 30) No.1, Type A, ℓA could be made more stable at low temperatures by turning it longer emulsifier in between Line A and Line B. (Refer to the temperature stability and correction of emulsion).

⑥Respective quantity ratios

Formulas are classified by their quantity ratios of O:W, OSAA:WSAA. (Table 6 is prepared on a typical formula making either of OSAA and WSAA as 1/10 of the quantities of oil phase and water phase.)

⑦Quantity ratios of emulsifier

This will become one of the main causes to determine to which formula number an emulsion formula belongs. Furthermore, the quantity of OSAA, WSAA shown in the column is a standard quantity and the quantity of OSAA, WSAA generally increases or decreases keeping the ratio.

⑧Quantity ratio and tendency of viscosity

It shows the relationship between the ratios of O:W, OSAA : WSAA and the viscosity of emulsifier. Determination of viscosity is based on the following:

0 : State of water 5: State of solution 10: Oily

15: State of soft milky lotion 20: State of milky lotion

25: State of soft cream 30: Creamy

⑨Tendency of dilution

"E" denotes emulsification, "S" solubilization and "/" separation. The table shows the tendency of each type to emulsify when diluted with water (Aq) or oil. The column of Rp SAA-Oil shows the tendency to emulsify when diluted with oil while the column of Rp SAA-Aq the tendency to emulsify when diluted with water (Aq). The column SAA increase in quantity indicates the tendency to emulsify when the quantity of SAA was increases by two to four times and each type of emulsion is diluted by water (Aq) or oil. (ii) Prediction of Properties

Development of New Formulas

3.4 Development of New Formulas

The design of emulsion formulas using the organic conceptual diagram has also proved to be useful for the development of new formulas. If the properties of intended emulsions and readily fixed ingredients as obtained from commodity planning were known, the intended emulsions could be efficiently obtained using the organic conceptual diagram and the tendency list of quality and quantity. In the emulsification test after ingredients were selected, the tendency of emulsion can be determined by taking the ratio of quantities of OSAA : WSAA as against oil phase: water phase in the same (ratio of quantities) as in the tendency list of quality and quantity.

If formulas are modified while confirming, the tendency in the change in the state of emulsification by combination of the change in the ratio of quantity of SAA and the tendency of selecting emulsifier, the intended emulsion could be developed in a shorter period of time. Introduced briefly below are the procedures for the development of new formulas using the organic conceptual diagram:

Procedure 1 Setting the Types of Emulsion According to Product Specifications

Generally, Type A emulsion, having a strong hydrophily, possesses high degreasing power, expansion and penetration actions. Because of these properties, Type A tends to be selected for emulsion aiming primarily at detergents. Furthermore, as the expansion and penetration actions of Type A emulsion cause injury and irritation of the skin, Type B is generally selected for basic cosmetics in consideration of safety.

Procedure 2 Selection of Quantity Ratio between Oil Phase and Water Phase, and Quantity of Emulsion

Respective quantities are provisionally determined from the required product specifications, in reference to the tendency list of quality and quantity.

Table 7 - Recommended types and formula numbers

Facial foam	Type A	ℓA	ℓ : 𝓈	(Formula No.5, 7, 8)
Cleansing oil	Type B	ℓB	ℓ : 𝓈	(Formula No.2)
Cleansing cream	Type B	ℓA	ℓ : 𝓈	(Formula No.2, 3)
Cleansing gel (large water phase quantity)	Type A	ℓA	ℓ : 𝓈	(Formula No.5, 8)
Cleansing gel (large oil phase quantity)	Type B		ℓ : 𝓈	(Formula No.2, 3)
Skin lotion	Type A	ℓA	ℓ : 𝓈	(Formula No.7)
Milky lotion	Type B	ℓA	ℓ : 𝓈	(Formula No.5, 6)
Cold cream	Type B	ℓA	ℓ : 𝓈	(Formula No.1, 2)
Sunscreen	Type B	ℓB	𝓈 : ℓ	(Formula No.6)
Body soap	Type A	ℓA		(Formula No.7)
Shampoo	Type A	ℓB		(Formula No.7)
Rinse	Type B	ℓA	ℓ : 𝓈	(Formula No.6)

Procedure 3 Selection of Emulsifier

Similarly with the provisional setting of quantity, pay careful attention to the elements characterizing formula (ℓA or ℓB, 𝓈 : ℓ or ℓ : 𝓈) and select the emulsifier from the organic conceptual diagram. Combinations of emulsifier favorably affect the stability of the emulsion in many formulas. However, the setting of the quantity ratio as a new parameter increases the number of emulsification tests.

In the design of emulsion formulas using the organic conceptual diagram, therefore, the initial test is conducted by allocating the ratio of mixing of each arbitrary emulsifier by geometrical progress of common ratio 2 from oil and Aq toward the emulsifier with the largest mix quantity (desired to be increased).(Fig.8, 9,10 and 11) Allocation should be made in equal quantity to those closely located on the same ratio line (same α). This is to determine the tendency of emulsion from formulas based on certain rules. Having a large influence on the properties of emulsion is rather the distance of emulsifiers (from the origin), it is necessary to carefully consider the distance in the selection of emulsifier from the organic conceptual diagram.

Procedure 4 Emulsification Test

Emulsification tests and evaluation are conducted in accordance with each parameter set.

Procedure 5 Correction of Formulas

It would be extremely rare to obtain intended emulsion by a single emulsification test and evaluation. For changing formula for retesting, the positional relationship of emulsifier over on the organic conceptual diagram and the tendency list of quality and quantity give a good prediction. In particular, with respect to the stability of emulsification at normal temperatures and stability against changes in temperature which becomes problematical, improvement will be made possible if emulsifier were reselected as follows from the organic conceptual diagram:

(i) Emulsification Stability

a. Carry out retests by changing one of the emulsifier in the formula to one at a different length (distance) on the same ratio line (Fig.14).

b. Increase the length of emulsifier agent close to either Line A or Line B.

(ii) Temperature Stability

Refer to the tendency list of quality and quantity and change the length of emulsifier used between Lines, A and B over the same ratio line. This enables determination of the relationship between the length of emulsifier and the tendency of temperature stability in the range -5 to 40˚C in the formula. Fig.15 shows the case of anionic surfactant(LineA~90˚). In case of nonionic surfactant, the tendency of distance is reversed. (Long = Stable at high temperature, short = stable at low temperature). By repeating the procedures the intended emulsion can be efficiently developed.

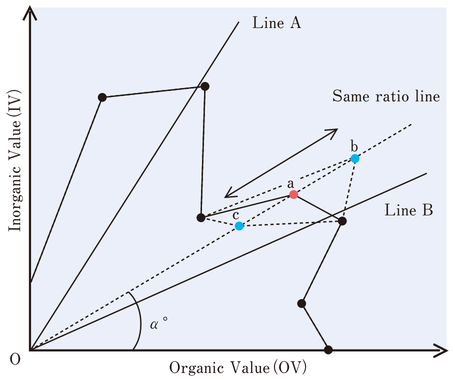


Fig.14 - Selection of emulsifier on the same ratio line

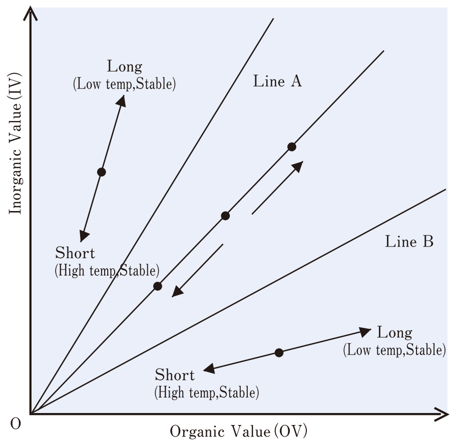


Fig.15 - Relationship between the distance of emulsifying agent and temperature stability

4 Examples of Execution

4.1 Assessment of Established Formula by the Organic Conceptual Diagram

Table 8 - Sample formula

Ingredients	wt%	OV	IV	Remarks	
㈰ Liquid Paraffin	28.55	300	0	Oil=28.55	O=35 (OSAA=6.45)
㈪ Cetyl Octanoate	0.9	470	60		
㈫ Cetanol	1.85	320	100		
㈬ POE(2) Stearyl ether (EMALEX 602)	3.7	440	195		
					Line B
㈭ POE(8) Distearate (EMALEX 400di-S)	0.85	1040	645		W=65 (WSAA=1.6)
㈮ POE(11) Stearyl ether (EMALEX 611)	0.4	800	870		
㈯ POE(20) Lauryl ether (EMALEX 720)	0.2	1040	1545		
					Line A
㉀ PEG-600	0.1	480	1025		
㈷ Sodium-stearoyl-glutamate	0.05	460	1000		
㉂ Purified Water	63.4	0	100		
	100.0				

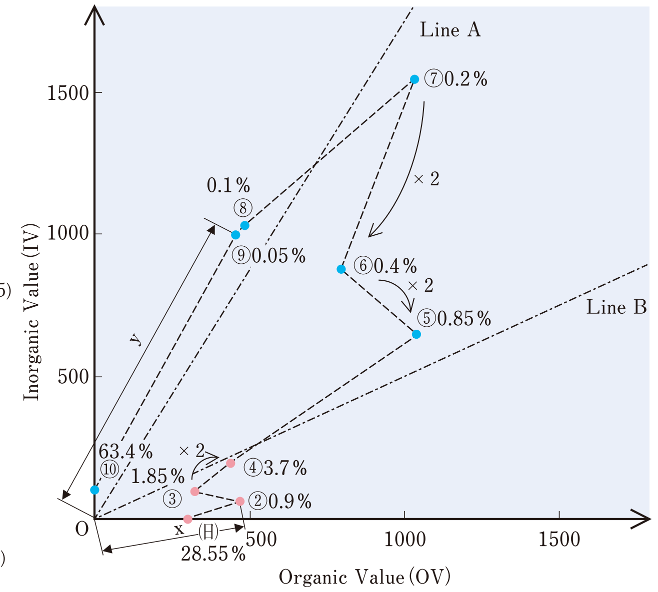


Fig.16 - Conceptual diagram of sample formula

Table 9 - Results of type assessment (No.6, Type B, ℓA, 𝓈 : ℓ)

Assessed items	Results	Reasons
Type A or B	Type B	Emulsifiers are found mostly in vicinity of Line B.
ℓA or ℓB	ℓA	The ingredient the furthest distance from the origin in the formula is ⑦POE(20) Lauryl ether (EMALEX 720) in vicinity of Line A
𝓈 : ℓ or ℓ : 𝓈	𝓈 : ℓ	The distance of the ingredient②, with the smallest α in oil phase ingredients is shorter than that of ingredients with the largest-⑨, in water phase ingredients.
O : W	O=35%	The sum of four ingredients within Line B from 0°
	W=65%	The sum of six ingredients from over Line B to water
Osaa : Wsaa	OSAA=6.45%	The sum of three ingredients of oil phase excluding liquid paraffin
	WSAA=1.6%	The sun of five ingredients of water phase excluding water
Formula number	6	From Appendix 2 / WSAA／OSAA=1.6／6.45=0.248 ⟶Formula No.6 B 35 : 65 (OSAA : WSAA 6.5 : 1.6) 1.6 : 6.5=0.246 approximate number
Predicted from the above is a cream in a state of soft cream stable at high temperature and with fresh feel leaving slightly whitish residue on application.		

4.2 Formula Development According to Product Specifications

The flow of the design of emulsion formula using the organic conceptual diagram is introduced taking massage cream as an example.

Specifications required of the products:

Massage cream with an excellent feel for massage, which will leave a moist sensatione even after rinsing.

①Setting of emulsion type ⇒ Type B emulsion

Reason: Safety for the skin and it is produced with oil since the product is a basic cosmetic applied to the skin.

②Ratio of oil phase quantity : water phase quantity ⇒ O : W = 65 : 35.

Reason: Formula No.1 ~ 4 in Appendix 2 since oil contents are high.

In the range of O : W = 85 : 15~50 : 50, the viscosity generally goes up at 70 : 30~65 : 35. To improve the oil contents and the feeling of massage, O : W = 65 : 35 was selected.

③Examination of the quantity of emulsifiers

OSAA : WSAA was selected from the "tendency list of quality and quantity (Appendix 2).

Selection of formula No. ⇒ No.2B. (OSAA : 6.5%, WSAA : 3.9%)

Reason: As the formula was desired to leave a moist feeling even after rinsing on completion of the massage.

In No.1B (OSAA : 6.5%, WSAA : 1.6%), the formula fails to re-emulsify at the time of rinsing, leaving the feel of too much oil residue. while in No.3B (OSAA : 3.9%, WSAA : 6.5%), No.4B (OSAA : 1.6%, WSAA : 6.5%), it rinses well, leaving very fresh feeling.

④Selection of emulsifier

No.2B, ℓA, ℓ : 𝓈, is chosen.

Reason: ℓA : To improve the suitability to (condition of) the skin on application and make it easy to rinse with running water after the massage.

ℓ : 𝓈 : To produce the feeling of emollient qualities after rinsing.

⑤Emulsification test and evaluation

Emulsification test and evaluation will be made in line with 2B, ℓA, ℓ : 𝓈, O : W = 65 : 35, OSAA:WSAA = 6.5:3.9.

⑥Correction of formula

Perform re-examination based on the tendency list.

(Refer to Chapter3.4㈭ "Temperature stability of emulsion and its correction").

5 Conclusion

This pamphlet outlines the design emulsion formulas using the organic conceptual diagram. This shows that formula studies can be efficiently accelerated by clarifying set conditions and correctly understanding the "tendency list of quality and quantity". The "design of emulsion formulas using the organic conceptual diagram" is not a strict science. It is, however, widely known in the cosmetics industry that this method has produced practical achievements in the development of many emulsion formulas. This pamphlet is only an introduction of the "design of emulsion formulas using the organic conceptual diagram". We will be more than happy if it proves useful to researchers in the study of formulas. It is our intention to continue our research, for further development in the "design of emulsion formulas using the organic conceptual diagram".

Appendix 1 - Organic and Inorganic Values

Inorganic radical	Inorganic value	Organic and inorganic values	Organic value	Inorganic value
Light metal	500<	R_4P-OH	20	250
Heavy metal, amine and NH_4 salt	400<	$-O-SO_3H$	20	220
$-SO_2-NH-CO-$, $-N=N-NH_2$	260	$>SO_2$	40	170
$\Rightarrow N^+-OH$, $-SO_3H$, $-NHSO_2-NH$	250	>SO	40	140
$\Rightarrow S-OH$, –CONH–CONH–COMH–, SO_2NH-	240	–CSOH, –COSH	80	80
–CONH–	200	$-NO_2$	70	70
→N→O	170	–As<, –CN	40	70
–COOH	150	–P<	20	70
Lactone cyclization	120	–NO	50	50
–CO–O–CO–	110	$-O-NO_2$	60	40
–OH	100	–NC	40	40
–NH–NH, –O–CO–O–	80	–P=P–, –NCO	30	30
–N< ($-NH_2$, –NHφ, $-N\phi_2$) amine	70	–O–NO, –SH, –S–	40	20
>CO	65	–I	80	10
–COOR, Naphthalene nucleus, Quinoline nucleus	60	–Br	60	10
>C=NH	50	=S	50	10
–O–O–	40	–Cl	40	10
–N=N–	30	–F	5	5
–O–	20	Iso branch >—	–10	0
Benzene nucleus (general aromatic monocycle), pyridine nucleus	15	Tert branch >—	–20	0
Ring (general non-aromatic monocycle)	10	>C<	20	0
$-(OCH_2CH_2)-$, Sugar ring–O–, under normal temperature, (Temp.>Cloud point)	75(20)	Triple bond	3	0
		Double bond	2	0

Appendix 2 - Tendency list of quality and quantity

Phase quantity	Formula No.	Type of emulsion	Selection tendency of surfactant	Temperature stability tendency of formula	Tendency of temperature stability and length: Line B~Line A (Nonion)	O : W 85 : 15	O : W 80 : 20	O : W 75 : 25	O : W 70 : 30	O : W 65 : 35	O : W 60 : 40	O : W 55 : 45	O : W 50 : 50
						$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$	$O_{SAA} : W_{SAA}$
O>W	1	A	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	8.5 : 0.8 (0.1) ↖(W_{SAA}/O_{SAA})	8.0 : 1.0 (0.1)	7.5 : 1.2 (0.2)	7.0 : 1.4 (0.2)	6.5 : 1.6 (0.2)	6.0 : 1.8 (0.3)	5.5 : 2.0 (0.4)	5.0 : 2.1 (0.4)
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
		B	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	3 / 5			10 / 30	26 / 30			20 / 28 / 25
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
	2	A	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	8.5 : 7.1 (0.8)	8.0 : 6.3 (0.8)	7.5 : 5.4 (0.7)	7.0 : 4.6 (0.7)	6.5 : 3.9 (0.6)	6.0 : 3.2 (0.5)	5.5 : 2.6 (0.5)	5.0 : 2.1 (0.4)
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
		B	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	14 / 12			25 / 30 / 20 / 28	23 / 30 / 28			20 / 28 / 25
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
	3	A	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	7.1 : 8.5 (1.2)	6.3 : 8.0 (1.3)	5.4 : 7.5 (1.4)	4.6 : 7.0 (1.5)	3.9 : 6.5 (1.7)	3.2 : 6.0 (1.9)	2.6 : 5.5 (2.1)	2.1 : 5.0 (2.4)
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
		B	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	12 / 15			23 / 26	17 / 24 / 28			5 / 15 / 10
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
	4	A	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	0.8 : 8.5 (10.6)	1.0 : 8.0 (8.0)	1.2 : 7.5 (6.3)	1.4 : 7.0 (5.0)	1.6 : 6.5 (4.1)	1.8 : 6.0 (3.3)	2.0 : 5.5 (2.8)	2.1 : 5.0 (2.4)
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
		B	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	5 / 10			20 / 29	14 / 18 / 25			5 / 15 / 10 (Visc.)
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
s↗ : Short for stability in high Temp. ℓ↙ : Long for stability in low Temp.						15 : 85	20 : 80	25 : 75	30 : 70	35 : 65	40 : 60	45 : 55	50 : 50
O<W	5	A	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	8.5 : 7.1 (0.8)	8.0 : 6.3 (0.8)	7.5 : 5.4 (0.7)	7.0 : 4.6 (0.7)	6.5 : 3.9 (0.6)	6.0 : 3.2 (0.5)	5.5 : 2.6 (0.5)	5.0 : 2.1 (0.4)
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
		B	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	18 / 20			21 / 17	23 / 25 / 28			20 / 28 / 25
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
	6	A	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	8.5 : 0.8 (0.1)	8.0 : 1.0 (0.1)	7.5 : 1.2 (0.2)	7.0 : 1.4 (0.2)	6.5 : 1.6 (0.2)	6.0 : 1.8 (0.3)	5.5 : 2.0 (0.4)	5.0 : 2.1 (0.4)
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
		B	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	22 / 20			25 / 8	23 / 25 / 28			20 / 28 / 25
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
	7	A	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	0.8 : 8.5 (10.6)	1.0 : 8.0 (8.0)	1.2 : 7.5 (6.3)	1.4 : 7.0 (5.0)	1.6 : 6.5 (4.1)	1.8 : 6.0 (3.3)	2.0 : 5.5 (2.8)	2.1 : 5.0 (2.4)
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
		B	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	0 / 5			3~6 / 9	6 / 13			5 / 15 / 10
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								
	8	A	ℓA ℓ : s / s : ℓ	↙	ℓ ↗ / ℓ ↗	7.1 : 8.5 (1.2)	6.3 : 8.0 (1.3)	5.4 : 7.5 (1.4)	4.6 : 7.0 (1.5)	3.9 : 6.5 (1.7)	3.2 : 6.0 (1.9)	2.6 : 5.5 (2.1)	2.1 : 5.0 (2.4)
			ℓB ℓ : s / s : ℓ	↙	s ↗ / s ↗								
		B	ℓA ℓ : s / s : ℓ	↗	ℓ ↙ / ℓ ↙	21 / 25			15 / 13	11 / 18 / 22			5 / 15 / 10
			ℓB ℓ : s / s : ℓ	↗	s ↙ / s ↙								

Tendency of temperature stability and length: Line B~Line A (Nonion)	Temperature stability tendency of formula	Selection tendency of surfactant	Type of emulsion	Formula No.	Phase quantity	Dilution tendency: RpSAA Oil	RpSAA Aq	SAA increase in quantity Oil	SAA increase in quantity Aq
s ↗ / s ↗	↙	ℓA ℓ : s / s : ℓ	A	1	O≧W	E	／	E	E
ℓ ↙ / ℓ ↙	↗	ℓB ℓ : s / s : ℓ							
s ↙ / s ↙	↗	ℓA ℓ : s / s : ℓ	B			E	／	E	E
ℓ ↗ / ℓ ↗	↙	ℓB ℓ : s / s : ℓ							
s ↗ / s ↗	↙	ℓA ℓ : s / s : ℓ	A	2		E	／	E	E
ℓ ↙ / ℓ ↙	↗	ℓB ℓ : s / s : ℓ							
s ↙ / s ↙	↗	ℓA ℓ : s / s : ℓ	B			S	／	S	E
ℓ ↗ / ℓ ↗	↙	ℓB ℓ : s / s : ℓ							
ℓ ↗ / ℓ ↗	↙	ℓA ℓ : s / s : ℓ	A	3		E	／	E	E
s ↙ / s ↙	↗	ℓB ℓ : s / s : ℓ							
ℓ ↙ / ℓ ↙	↗	ℓA ℓ : s / s : ℓ	B			S	／	S	E
s ↗ / s ↗	↙	ℓB ℓ : s / s : ℓ							
ℓ ↗ / ℓ ↗	↙	ℓA ℓ : s / s : ℓ	A	4		E	／	E	E
s ↙ / s ↙	↗	ℓB ℓ : s / s : ℓ							
ℓ ↙ / ℓ ↙	↗	ℓA ℓ : s / s : ℓ	B			E	／	E	E
s ↗ / s ↗	↙	ℓB ℓ : s / s : ℓ							
Viscosity of emulsion (Visc.) 0: State of water 5: State of solution 10: Oily 15: State of soft milky lotion 20: State of milky lotion 25: State of soft cream 30: Creamy									
s ↗ / s ↗	↙	ℓA ℓ : s / s : ℓ	A	5	O≦W	／	S	E	S
ℓ ↙ / ℓ ↙	↗	ℓB ℓ : s / s : ℓ							
s ↙ / s ↙	↗	ℓA ℓ : s / s : ℓ	B			／	E	E	E
ℓ ↗ / ℓ ↗	↙	ℓB ℓ : s / s : ℓ							
s ↗ / s ↗	↙	ℓA ℓ : s / s : ℓ	A	6		／	E	E	E
ℓ ↙ / ℓ ↙	↗	ℓB ℓ : s / s : ℓ							
s ↙ / s ↙	↗	ℓA ℓ : s / s : ℓ	B			／	E	E	E
ℓ ↗ / ℓ ↗	↙	ℓB ℓ : s / s : ℓ							
ℓ ↗ / ℓ ↗	↙	ℓA ℓ : s / s : ℓ	A	7		／	E	E	E
s ↙ / s ↙	↗	ℓB ℓ : s / s : ℓ							
ℓ ↙ / ℓ ↙	↗	ℓA ℓ : s / s : ℓ	B			／	E	E	E
s ↗ / s ↗	↙	ℓB ℓ : s / s : ℓ							
ℓ ↗ / ℓ ↗	↙	ℓA ℓ : s / s : ℓ	A	8		／	S	E	S
s ↙ / s ↙	↗	ℓB ℓ : s / s : ℓ							
ℓ ↙ / ℓ ↙	↗	ℓA ℓ : s / s : ℓ	B			／	E	E	E
s ↗ / s ↗	↙	ℓB ℓ : s / s : ℓ							

E : Emulsification
S : Solbilization
／ : Separation