

Supplementary

1. HLB calculated of Surfactants

1.1. Non-ionic Surfactant

For no-ionic surfactants, the HLB values of individual surfactant molecules can be calculated applying the Griffin formula [1]:

$$HLB = \frac{20 \times MW_H}{MW_H + MW_L}$$

Where, MW_H = molar weight of hydrophilic portion and MW_L = molar weight of hydrophobic portion.

*Lauryl glucoside HLB:

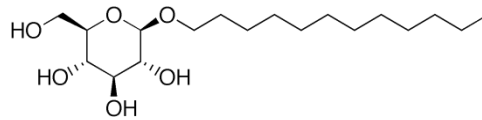


Figure. 1. Chemical structure of Lauryl glucoside

$$\begin{aligned} \text{Hydrophilic portion} &= MW_{(C_6H_{11}O_6)} = (12.01 \times 6) + (1.01 \times 11) + (16.00 \times 6) \\ &= 179.15 \text{ Da} \end{aligned}$$

$$\text{Hydrophobic portion} = MW_{(C_{12}H_{25})} = (12.01 \times 12) + (1.01 \times 25) = 169.32 \text{ Da}$$

$$\text{HLB Lauryl Glucoside} = \frac{20 \times 179.15}{179.15 + 169.32} = \mathbf{10}$$

1.2. Cationic Surfactants

For ionic surfactants, the HLB values of individual surfactant molecules can be calculated applying the Davies formula [2]:

$$HLB = \sum (\text{Hydrophilic group contributions}) - \sum (\text{Hydrophobic group contributions}) + 7$$

Hydrophilic and hydrophobic group values are taken from the Davies tables [3].

***Hydroxyethyl-Behenamidopropyl-Diammonium Chloride (HBDC) HLB:**

$$HLB_{HBDC} = (22.0 + 9.4 + 2.1 + 1.9) - (24 \times 0.475) + 7 = 31$$

*** Behentrimonium Methosulphate (BT-MS) HLB:**

$$HLB_{BT-MS} = (22.0) - (22 \times 0.475) + 7 = 19$$

*** Cetrimonium Chloride (CT-Cl) HLB:**

$$HLB_{CT-Cl} = (22.0) - (15 \times 0.475) + 7 = 22$$

***Polyquaternium 70 (PQ70) HLB:**

$$HLB_{PQ70} = (22 + 2.1 + 2.1 + 1.3 \times 8 + 1.9) - (69 \times 0.475) + 7 = 13$$

1.3. Surfactants mixtures

System 1

$$HBD - Cl: BT - MS (1: 3) = \frac{(31 \times 0.25) + (19 \times 0.75) + (10 \times 0.2)}{1.2} = 20$$

System 2

$$HBD - Cl: BT - MS (1: 1) = \frac{(31 \times 0.5) + (19 \times 0.5) + (10 \times 0.2)}{1.2} = 23$$

System 3

$$HBD - Cl: BT - MS (3: 1) = \frac{(31 \times 0.75) + (19 \times 0.25) + (10 \times 0.2)}{1.2} = 25$$

System 4

$$HBD - Cl: CT - Cl (1: 3) = \frac{(31 \times 0.25) + (22 \times 0.75) + (10 \times 0.2)}{1.2} = 22$$

System 5

$$HBD - Cl: CT - Cl (1: 1) = \frac{(31 \times 0.5) + (22 \times 0.5) + (10 \times 0.2)}{1.2} = 24$$

System 6

$$HBD - Cl: CT - Cl (3: 1) = \frac{(31 \times 0.75) + (22 \times 0.25) + (10 \times 0.2)}{1.2} = 26$$

System 7

$$HBD - Cl: PQ - 70(1: 3) = \frac{(31 \times 0.25) + (13 \times 0.75) + (10 \times 0.2)}{1.2} = 16$$

System 8

$$HBD - Cl:PQ - 70(1:1) = \frac{(31 \times 0.5) + (13 \times 0.5) + (10 \times 0.2)}{1.2} = \mathbf{20}$$

System 9

$$HBD - Cl:PQ - 70(3:1) = \frac{(31 \times 0.75) + (13 \times 0.25) + (10 \times 0.2)}{1.2} = \mathbf{24}$$

System 10

$$BT - MS:CT - Cl (1:3) = \frac{(19 \times 0.25) + (22 \times 0.75) + (10 \times 0.2)}{1.2} = \mathbf{19}$$

System 11

$$BT - MS:CT - Cl (1:1) = \frac{(19 \times 0.5) + (22 \times 0.5) + (10 \times 0.2)}{1.2} = \mathbf{19}$$

System 12

$$BT - MS:CT - Cl (3:1) = \frac{(19 \times 0.75) + (22 \times 0.25) + (10 \times 0.2)}{1.2} = \mathbf{18}$$

System 13

$$BT - MS:PQ - 70 (1:3) = \frac{(19 \times 0.25) + (13 \times 0.75) + (10 \times 0.2)}{1.2} = \mathbf{14}$$

System 14

$$BT - MS:PQ - 70 (1:1) = \frac{(19 \times 0.5) + (13 \times 0.5) + (10 \times 0.2)}{1.2} = \mathbf{15}$$

System 15

$$BT - MS:PQ - 70 (3:1) = \frac{(19 \times 0.75) + (13 \times 0.25) + (10 \times 0.2)}{1.2} = \mathbf{16}$$

System 16

$$CT - Cl:PQ - 70 (1:3) = \frac{(22 \times 0.25) + (13 \times 0.75) + (10 \times 0.2)}{1.2} = \mathbf{14}$$

System 17

$$CT - Cl:PQ - 70 (1:1) = \frac{(22 \times 0.5) + (13 \times 0.5) + (10 \times 0.2)}{1.2} = \mathbf{16}$$

System 18

$$CT - Cl:PQ - 70 (3:1) = \frac{(22 \times 0.75) + (13 \times 0.25) + (10 \times 0.2)}{1.2} = \mathbf{18}$$

2. Required HLB of oil phase

Required HLB from each component of the oil phase were taking from literature [4–6], and the required HLB of the total oil phase was calculated using Griffin formula [1]:

$$HLB_{required} = \sum HLB_{required_i} \times f_i$$

Were f_i is the mass or weight fraction of the oil i .

Due to the above, the required HLB of the oil phase used in this formula is:

Ingredient	% (w/w)	Required HLB
Cetearyl-alcohol	4.0	13.2 [4]
Coco-caprylate	0.5	9.3 [5]
Shea butter	0.3	7.0 [6]

$$HLB_{required} = \left(\frac{(13.2 \times 4) + (9.3 \times 0.5) + (7 \times 0.3)}{4.8} \right) = \mathbf{12.4}$$

References

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