# Surfactant Spectator

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Surfactant Spectator is electronic newsletters in the field of Surfactant Chemistry, placed on the web four times a year. We welcome comments, articles and information on the content of this newsletter.


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**Editor's note:**

Surfactants are very important materials used in many applications. **The Surfactant Spectator**® is a downloadable newsletter that addresses topics of interest to the formulator using surfactants.

This first edition of **The Surfactant Spectator**® offers two articles which are important to the reader. They are:

FIRP BOOKLET # E300-A

Green Star Rating® for Raw Materials and Formulations

The first an outstanding review of surfactant chemistry and the latter an approach to a topic of great concern today, namely a system to evaluate the environmental impact of surfactants as raw materials and as formulated products.

To download the booklet in pdf format click on the box below:

FIRP BOOKLET # E300-A

The article Green Star Rating® for Raw Materials and Formulations is presented below.

**The Surfactant Spectator**® solicits articles from members of the technical community for publication.

**Thomas G. O'Lenick Editor**

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# Green Star Rating for Raw Materials and Formulations


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Today's consumer and formulator have become increasingly aware of the consumption of resources that are not renewable. Products derived from fossil fuels are nonrenewable. This includes products like gasoline, coal, natural gas, diesel, and other commodities. Green resources are defined as renewable resources, which can be replenished by natural processes. Green products are renewable resources include oxygen, fresh water, timber, and biomass. Green products also include commodities such as wood, paper, and leather. Furthermore, alcohol, oils from plants and seeds are considered green products.

These green raw materials are more environmental friendly than their non-renewable counter parts and minimize the negative impact on the earth. However, these basic green products cannot be combined in a way to provide consumer products that meet the demands of the consumer. For example, soap can be a green detergent but it does not possess all the desirable properties that give the consumer a laundry detergent. In order to make high performance formulations, some materials that are not 'green' are required.

While the concept of green products is straightforward, the ability for the formulator and the consumer to quantify the greenness of a given shampoo or other consumer product is elusive. Given a proper understanding, the consumer and formulator can make better informed and better educated decisions about the best combination of green properties and formulation attributes for their products. In other words, the need of the consumer and the need of the environment can be intelligently determined.

All too often, the determination of the greenness of a raw material or formulation is more an emotional rather than a scientific decision and requires either an all or noting approach to environmental stewardship. Simply put, materials are either green or they are not. Unfortunately, the formulation of consumer products that are commercially acceptable require a trade off in optimizing the performance and greenness. The consumers demand for many formulation benefits cannot be achieved with all green ingredients, therefore, "non-green" products are required. The consumer then needs a systematic approach to develop a measurable metric for the level of greenness in a formulation and trade off some greenness for performance. This quest has resulted in the development of "Green Star Rating" system or simply "GSR".

The Green Star Rating provides a process by which a formulator can easily ascertain the "greenness" of a raw material and as importantly, a consumer can determine and compare the "greenness" of a formulation to similar types of products. This process allows the formulation chemist a way to break a molecule down into green portion and the not-green (or non-renewable) portion. The evaluation of this data leads to the generation of a Green Star Value, which is the percentage of the molecule that is based upon green chemistry. The Green Star Rating is found by taking the Green Star Value and multiplying it by the amount of active in the raw material (% solids). To obtain the Green Star Rating for a formulation, simple add up the contributions by each of the raw materials. Once this number is known, the effect of replacing one ingredient in a formulation with a "greener" compound can be ascertained. Specifically, if a raw material used in a formulation at 20% by weight has a Green Star Rating of 1 is replaced with a product with a Green Star Rating of 7, the impact on the formulation is (7-1) times 0.20 or 1.2. This means that much more renewable resources are being used in the formulation and its consumption of this product will have less of a negative impact on the environment. This approach allows the formulator to make greener product, those with a higher Green Star Rating, and the consumer to choose these greener products.

The Green Star Rating is determined using the following steps:

(1) Determining the empirical formula for chemical compounds used to make formulated products,

(2) Determining which portions of the molecule are green;

(3) Determining the percentage by weight of the green portion of the molecule;

(4) Determining the green star value

and optionally

(5) Optimizing the formulation by selecting components with the greatest green star value.

**Raw Materials**

**Example 1 - Sodium Coco Alcohol Derived From Natural Alcohol**

**Step one -** determining the empirical formula for chemical compounds used to make formulated product:

Example – Sodium Coco sulfate

$C_{12}H_{23}SO_4Na$

**Step two –** determining which portions of the molecule are green;

Example – Sodium coco sulfate

Renewable Material Natural Alcohol $C_{12}H_{23}$

Non-Renewable Synthetic Sulfation $SO_4Na$

**Step three** – determining the percentage by weight of the green portion of the molecule. This is done by multiplying the weight of each atom by the number of atoms of in each portion

Renewable - Natural Alcohol $C_{12}H_{23}$

Carbon has a molecular weight of 12 there are 12 present in the renewable portion so the molecular weight contribution of the carbon is 12 times 12 or 144.

Hydrogen has a molecular weight of 1 there are 23 hydrogen atoms present in the renewable portion so the molecular weight contribution of the hydrogen is 1 times 23 or 23.

The sum of all the elements in the renewable portion is 144+23 or 167.

The Non-renewable portion is $SO_4Na$.

Sulfur has a molecular weight of 32 there is 1 sulfur atom present in the non-renewable portion so the molecular weight contribution of the sulfur is 1 times 32 or 32.

Oxygen has a molecular weight of 16 there are 4 oxygen atoms present in the non-renewable portion so the molecular weight contribution of the hydrogen is 4 times 16 or 64.

Sodium has a molecular weight of 23 there is 1 sodium atom present in the non-renewable portion so the molecular weight contribution of the sulfur is 1 times 23 or 23.

The sum of all the elements in the non-renewable portion is 32+64+23= 119

Total Molecular Weight = Renewable Portion + Non-Renewable portion

Total Molecular Weight = 167+ 119= 289

Renewable Portion/ Total = 167/289 = 57.7%

Step 4 determining the Green Star Value

Green Star Value (GSV)= % Renewable rounded to unit = 58

**Raw Material Example 2** Sodium laureth 3 Sulfate

$C_{12}H_{23}O(CH_2CH_2O)_3SO_3Na$

Empirical Formula: $C_{18}H_{35}O_7SNa$

| | | | |
|---|---|---|---|
| Renewable | $C_{12}H_{23}$ | Synthetic | $-(CH_2CH_2O)_3SO_4Na$ |
| | Natural Alcohol | | EO-Sulfate |

Calculations

Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 12 | 23 | 0 | 0 | 0 | 0 | 0 | 0 |
| MW of atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 144.12 | 23.23 | 0 | 0 | 0 | 0 | 0 | 0 |
| Total MW | 167.35 | | | | | | | |

Non-Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 6 | 12 | 0 | 7 | 0 | 0 | 1 | 0 |
| MW of atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 72.06 | 12.12 | 0 | 111.93 | 0 | 0 | 22.98 | 0 |
| Total MW | 219.09 | | | | | | | |

| | |
|---|---|
| Total | 386.44 |
| % Renewable | 43% |
| Green Star Value | 43 |

Raw Material Example 3  Sodium Lauryl Sulfate (Ziegler Alcohol derived)

Example – Sodium lauryl sulfate

$$C_{12}H_{23}SO_4Na$$

**Step two –** determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

Example – Sodium lauryl sulfate

Synthetic  $C_{12}H_{23}\ SO_4Na$

**Step three –**

Renewable Portion

| | C | H | N | O | P | S | Na |
|---|---|---|---|---|---|---|---|
| Number of Atoms | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 |
| Number x MW | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Total | 0 | | | | | | |

Non-renewable Portion

| | C | H | N | O | P | S | Na |
|---|---|---|---|---|---|---|---|
| Number of Atoms | 12 | 23 | 0 | 4 | 0 | 1 | 1 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 |
| Number x MW | 144.12 | 23.23 | 0 | 63.96 | 0 | 32.01 | 22.98 |
| Total | 286.3 | | | | | | |

| | |
|---|---|
| Total | 286.3 |
| % Renewable | 0 |
| Green Star Value | 0 |

Raw Material Example 4  Cocamidopropyl Betaine

Structure

$$C_{11}H_{23}C(O)\text{-}N(H)\text{-}(CH_2)_3\text{-}\overset{\displaystyle CH_3}{\underset{\displaystyle CH_3}{N^+}}\text{-}CH_2C(O)\text{-}O^-$$

Formula  $C_{18}H_{38}O_3N_2$

**Step two –** determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

Renewable $C_{12}H_{23}O$ Nonrenewable $C_6H_{14}O_2N_2$

**Step three –**

Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 12 | 23 | 0 | 1 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 144.12 | 23.23 | 0 | 15.99 | 0 | 0 | 0 | 0 |
| Total | 183.34 | | | | | | | |

Non- Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number | 6 | 14 | 2 | 2 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 72.06 | 14.14 | 28.02 | 31.98 | 0 | 0 | 0 | 0 |
| Total | 146.2 | | | | | | | |

| | |
|---|---|
| Total | 329.54 |
| % Renewable | 55.6% |
| Green Star Value | 56 |

**Raw Material Example 5 – Cocamid DEA**

Structure $C_{11}H_{23}$-C(O)-N-$(CH_2CH_2OH)_2$

$C_{16}H_{30}O_3N$

**Step two –** determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

$C_{11}H_{23}$-C(O)-N-$(CH_2CH_2OH)_2$

Renewable $C_{12}H_{23}O$ Non-renewable $C_4H_{10}O_2N$

**Step three –**

Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 12 | 23 | 0 | 1 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 144.12 | 23.23 | 0 | 15.99 | 0 | 0 | 0 | 0 |
| Total | 183.34 | | | | | | | |

Non-Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number | 4 | 10 | 1 | 2 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 48.04 | 10.1 | 14.01 | 31.98 | 0 | 0 | 0 | 0 |
| Total | 104.13 | | | | | | | |

| | |
|---|---|
| Total | 287.47 |
| % Renewable | 63.8% |
| Green Star Value | 64 |

**Raw Material Example 6 – Cocamid MEA ($C_{14}H_{29}O_2N$)**

Structure $C_{11}H_{23}$-C(O)-NH-$CH_2CH_2OH$

**Step two –** determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic

$C_{11}H_{23}$-C(O)-NH$CH_2CH_2OH$

Renewable $C_{12}H_{23}O$ Non-renewable $C_2H_6ON$

**Step three –**

Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 12 | 23 | 0 | 1 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 144.12 | 23.23 | 0 | 15.99 | 0 | 0 | 0 | 0 |
| Total | 183.34 | | | | | | | |

Non- Renewable Portion

| | C | H | N | O | P | S | Na | K |
|---|---|---|---|---|---|---|---|---|
| Number of Atoms | 2 | 6 | 1 | 2 | 0 | 0 | 0 | 0 |
| MW of Atom | 12.01 | 1.01 | 14.01 | 15.99 | 30.97 | 32.01 | 22.98 | 39.1 |
| Number x MW | 24.02 | 6.06 | 14.01 | 31.98 | 0 | 0 | 0 | 0 |
| Total | 76.07 | | | | | | | |

| | |
|---|---|
| Total | 259.41 |
| % Renewable | 70.7% |
| Green Star Value | 71 |

**Formulations**

The Green Star Process can also be used on any formulation .\

**Conditioning Shampoo**

| | %weight |
|---|---|
| Water | 55.0 |
| Sodium Lauryl Sulfate | 18.0 |
| Sodium Laureth 3 Sulfate | 16.0 |
| Cocamidopropyl Betaine | 8.0 |
| Cocamid DEA | 3.0 |

**Example 7 Conditioning Shampoo (Version 1)**

This product is based on sodium lauryl sulfate (synthetic alcohol)

| | % weight | % solids | Example | GSV | Contribution | |
|---|---|---|---|---|---|---|
| Water | 55 | - | - | - | - | |
| Sodium lauryl Sulfate | 34 | 9.5 | Example 3 | 0 | 0 | (0.095 x 0) |
| Cocamidopropyl Betaine | 8 | 2.8 | Example 4 | 56 | 1.57 | (0.028 x 56) |
| Cocamid MEA | 3 | 3 | Example 6 | 71 | 2.13 | (0.03 x 71) |
| | | | | Total | 3.70 | |

**Example 8 Conditioning Shampoo (Version 2)**

This product is based on sodium lauryl sulfate (synthetic alcohol) and SLES-3

| | % weight | % solids | Example | GSV | Contribution | |
|---|---|---|---|---|---|---|
| Water | 55 | - | - | - | - | |
| Sodium Lauryl Sulfate | 17 | 4.5 | Example 3 | 0 | 0 | (.045 x 0) |
| Sodium Laureth 3 Sulfate | 17 | 4.5 | Example 2 | 43 | 1.94 | (.045 x 43) |
| Cocamidopropyl Betaine | 8 | 2.8 | Example 4 | 56 | 1.57 | (.028 x 56) |
| Cocamid DEA | 3 | 3 | Example 5 | 63 | 1.89 | (0.03 x 63) |
| | | | | Total | 5.39 | |

**Example 9 Conditioning Shampoo (Version 3)**

This product is based on sodium coco sulfate (renewable alcohol)

| | % weight | % solids | Example | GSV | Contribution | |
|---|---|---|---|---|---|---|
| Water | 55 | - | - | - | - | |
| Sodium Coco Sulfate | 17 | 4.5 | Example 1 | 58 | 2.61 | (.045 x 58) |
| Sodium Laureth 3 Sulfate | 17 | 4.5 | Example 2 | 43 | 1.94 | (.045 x 43) |
| Cocamidopropyl Betaine | 8 | 2.8 | Example 4 | 56 | 1.57 | (.028 x 56) |
| Cocamid DEA | 3 | 3 | Example 5 | 63 | 1.89 | (0.03 x 63) |
| | | | | Total | 8.00 | |

**Example 10 Conditioning Shampoo (Version 4)**

This product is based on sodium coco sulfate (renewable alcohol)

| | % weight | % solids | Example | GSV | Contribution | |
|---|---|---|---|---|---|---|
| Water | 55 | - | - | - | - | |
| Sodium Coco Sulfate | 17 | 4.5 | Example 1 | 58 | 2.61 | (.045 x 58) |
| Sodium Laureth 3 Sulfate | 17 | 4.5 | Example 2 | 43 | 1.94 | (.045 x 43) |
| Cocamidopropyl Betaine | 8 | 2.8 | Example 4 | 56 | 1.57 | (.028 x 56) |
| Cocamid MEA | 3 | 3 | Example 6 | 71 | 2.13 | (0.03 x 71) |
| | | | | Total | 8.24 | |

The simple formulations above show the power of the new system. Minor changes in the formulation made be properly selecting raw materials result in a 2.2 times improvement in the green star rating. This process allows the formulator to fine tune formulations to maximize greenness and to inform the consumer about the degree amount of a given formulation that is renewable. The same approach works not only on shampoos but also on all formulations.

| Example | Green Star Rating |
|---|---|
| 7 | 3.7 |
| 8 | 5.5 |
| 9 | 8.0 |
| 10 | 8.2 |

Conclusion

The Green Star Rating System provides the formulator and consumer with a metric by which both formulations and raw materials can be evaluated. The determination allows the consumer to pick the product with the *highest Green Star Rating that provides the attributes that customer demands*. Inherent in this system is the belief that consumers can make educated selections of cosmetic formulations that balance the desire for green products and at the same time answer all the consumer's demands vis-à-vis performance.

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