CHAPTER 5

Green Star Rating for Cosmetic Compounds and Formulations

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ABSTRACT: *The following is taken from U.S. Patent Application 20090259409, which directed toward "a process that can be used in the formulation of more environmentally friendly, greener formulations for consumer applications. The process includes evaluating the components in a formulation, then determining the percentage of the molecule that is green, establishing a green star rating and determining the effect of that component on the overall green star rating of a formulation."*

Background

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, replenished by natural processes. Green products are renewable resources and include oxygen, fresh water, timber and biomass (renewable energy source—biological material derived from living organisms). Green

products also include commodities such as wood, paper and leather. Furthermore, alcohol, oils from plants and seeds are considered green products.

Green raw materials are preferred in the preparation of cosmetic products, as they are both renewable and biodegradable. However, these basic green products cannot be combined in a way that provides 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 a green product is straightforward, the ability for the formulator and the consumer to quantify the greenness of a given shampoo or other consumer product is more difficult. Given a proper understanding, the consumer and formulator can make informed, educated decisions about creating products with the best combination of green properties and formulation attributes. In other words, the need of the consumer and the need of the environment can be intelligently determined.

All too often in the past, the determination of the greenness of a raw material or formulation was more emotional than scientific and required either an all or nothing approach to environmental stewardship. Simply put, materials are green or they are not. Unfortunately, the formulations of consumer products that are commercially acceptable require a trade-off in optimizing the performance and greenness. Consumers demand many formulation benefits that cannot be achieved with only green ingredients. Some non-green products are required. To educate the consumer, a systematic approach to measure the level of greenness in a formulation was needed. This quest resulted in the development of the "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 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 a

non-renewable resource portion. The evaluation of this data allows for the generation of a Green Star Value, which is the percentage of the molecule that is based upon green chemistry divided by 10. 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 with 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 will have less of a negative impact on the environment. This approach allows the formulator to make greener products and the consumer to choose greener products.

The Green Star Rating is determined using the following steps:

Step 1 Determine the empirical formula for chemical compounds used to make formulated products;

Step 2 Determine which portions of the molecule are green;

Step 3 Determine the percentage by weight of the green portion of the molecule;

Step 4 Determine the green star value and, optionally;

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

Raw Materials

There are two areas in which the Green Star Rating process can be applied: 1) to raw materials to allow for the prudent selection of products for inclusion into formulations, and to formulations themselves allowing for the generation of a Green Star Rating, a method for the consumer to understand the relative degree of greenness in a finished product.

Example 1—Sodium Coco Alcohol Derived from Natural Alcohol

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.

Sodium Coco Sulfate C12H23SO4Na

Step 2—Determine which portions of the molecule are green.

Sodium coco sulfate

Renewable Material	Natural Alcohol	C12H23
Non-Renewable	Synthetic Sulfation	SO_4Na

Step 3—Determine 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 in each portion.

Renewable Material	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.

Non-Renewable	Synthetic Sulfation	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—Determine the Green Star Value.
Green Star Value (GSV) = % Renewable rounded to unit = 58

Example 2—Sodium Laureth 3 Sulfate,
$C_{12}H_{23}O(CH_2CH_2O)_3SO_3Na$

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.

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

Step 2—Determine which portions of the molecule are green.

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

Step 3—Determine 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 in each portion.

Calculations

Renewable Portion								
	C	H	N	O	P	S	Na	K
Number	12	23	0	0	0	0	0	0
MW	144	23	0	0	0	0	0	0
Total	167							

Non- Renewable								
	C	H	N	O	P	S	Na	K
Number	6	12	0	7	0	0	1	0
MW	72	12	0	112	0	0	23	0
Total	219							

Total	386
% Renewable	43
Green Star Rating	43

Example 3—Sodium Lauryl Sulfate (Ziegler Alcohol derived)

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.

Sodium lauryl sulfate $C_{12}H_{23}SO_4Na$

Step 2—Determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

Non-renewable (Synthetic) $C_{12}H_{23}\,SO_4Na$

Step 3—Determine 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 in each portion.

Calculations

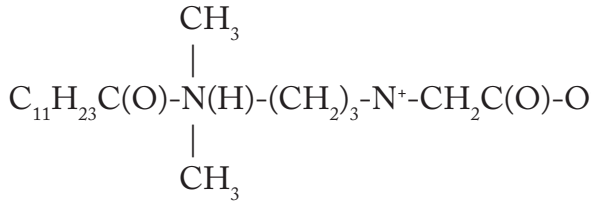
Renewable Portion								
	C	H	N	O	P	S	Na	K
Number	0	0	0	0	0	0	0	0
MW	0	0	0	0	0	0	0	0
Total	0							

Non- Renewable							
	C	H	N	O	P	S	Na
Number	12	23	0	4	0	1	1
MW	144	23	0	64	0	31	23
Total	285						

Total	285
% Renewable	0
Green Star Rating	0

Example 4—Cocamidopropyl Betaine

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.



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

Step 2—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 3—Determine 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 in each portion.

Calculations

Renewable Portion								
	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Non- Renewable								
	C	H	N	O	P	S	Na	K
Number	6	14	2	2	0	0	0	0
MW	72	14	28	32	0	0	0	0
Total	146							

Total	329
% Renewable	55.6
Green Star Rating	56

Example 5—Cocamid DEA

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.

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

$$C_{16}H_{30}O_3N$$

Step 2—Determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

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

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

Step 3—Determine 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 in each portion.

Calculations

	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Synthetic

	C	H	N	O	P	S	Na	K
Number	4	10	1	2	0	0	0	0
MW	48	10	14	32	0	0	0	0
Total	104							

Total	287
% Renewable	63
Green Star Rating	63

Example 6—Cocamid MEA

Step 1—Determine the empirical formula for chemical compounds used to make formulated product.

$$C_{11}H_{23}\text{-}C(O)\text{-}NH\text{-}CH_2CH_2OH$$
$$C_{14}H_{29}O_2N$$

Step 2—Determine which parts of the molecule are natural (derived from green natural raw materials) and which are synthetic.

$$C_{11}H_{23}\text{-}C(O)\text{-}NHCH_2CH_2OH$$

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

Step 3—Determine 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 in each portion.

Calculations

Renewable Portion

	C	H	N	O	P	S	Na	K
Number	12	23	0	1	0	0	0	0
MW	144	23	0	16	0	0	0	0
Total	183							

Non- Renewable

	C	H	N	O	P	S	Na	K
Number	2	6	1	2	0	0	0	0
MW	24	6	14	32	0	0	0	0
Total	76							

Total	259
% Renewable	70.6
Green Star Rating	71

Formulations

The Green Star Rating System can also be used on any formulation. All of the individual components in the formulation are rated and the overall Green Star rating is established.

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 1 Conditioning Shampoo

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

Ingredient	%weight	% Solids	Example	GRS	Contribution
Water	55.0	-	-	-	-
Sodium Lauryl Sulfate	34.0	9.5	3	0	0 (.095 times 0)
Cocamidopropyl Betaine	8.0	2.8	4	56	1.6 (.028 times 56)
Cocamid MEA	3.0	3.0	6	71	2.1 (.03 times 71)

Total 3.7

Example 2 Conditioning Shampoo (Version 1)

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

Ingredient	%weight	% Solids	Example	GRS	Contribution
Water	55.0	-	-	-	-
Sodium Lauryl Sulfate	17.0	4.5	3	0	0 (.045 times 0)

Sodium Laureth 3 Sulfate	17.0	4.5	2	43	2.0 (.045 times 43)
Cocamidopropyl Betaine	8.0	2.8	4	56	1.6 (.028 times 56)
Cocamid DEA	3.0	3.0	5	63	1.9 (.03 times 63)

Total 5.5

Example 3 Conditioning Shampoo

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

Ingredient	**%weight**	**% Solids**	**Example**	**GRS**	**Contribution**
Water	55.0	-	-	-	-
Sodium Coco Sulfate	17.0	4.5	1	58	2.6 (.045 times 58)
Sodium Laureth 3 Sulfate	17.0	4.5	2	43	1.9 (.045 times 43)
Cocamidopropyl Betaine	8.0	2.8	4	56	1.6 (.028 times 56)
Cocamid DEA	3.0	3.0	5	63	1.9 (.03 times 63)

Total 8.0

Example 4 Conditioning Shampoo

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

Ingredient	**%weight**	**% Solids**	**Example**	**GRS**	**Contribution**
Water	55.0	-	-	-	-
Sodium Coco Sulfate	17.0	4.5	1	58	2.6 (.045 times 58)
Sodium Laureth 3 Sulfate	17.0	4.5	2	43	1.9 (.045 times 43)
Cocamidopropyl Betaine	8.0	2.8	4	56	1.6 (.028 times 56)
Cocamid MEA	3.0	3.0	6	71	2.1 (.03 times 71)

Total 8.2

These simple formulations show the power of the new system. Minor changes in the formulation made by 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 amount of a given formulation that is renewable. The same approach works not only on shampoos but all formulations.

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 for the consumer to pick the product with the *highest Green Star Rating that provides the attributes consumers demand*. 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 about performance.