doctora liliana cosmetics

3/29/2023

A YELLOW AVOBENZONE COMPLEX

LILI'S NEW CHEM

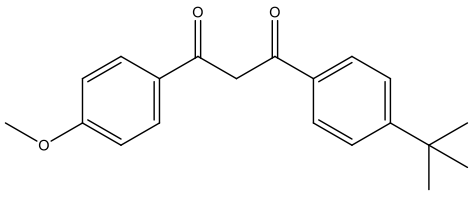
ON YELLOW COLORED PIGMENTS/DYES FROM AVOBENZONE ACCORDING TO LILI'S PENDING PATENTS[1]

"¿Qué será lo que fabricas tú?"

Amarillo by Shakira

Today, lili would like to present lili's new yellow complexes based on avobenzone.

Avobenzone, CAS 70356-09, or butyl methoxy dibenzoylmethane (Fig. 1) is a derivative of 1,3-diketone or β-diketone i.e., compounds which are like "the frame of glasses with antennas" such as lili told you in her post about avobenzone. [2] As a mentioned in that post, avobenzone can induce allergic reactions since avobenzone is absorbed into the body once is used and suffers from instability against solvents, light and more.



1-(4-tert-butylphenyl)-3-(4-methoxyphenyl)propane-1,3-dione

Fig. 1: Chemical structure of avobenzone

Avobenzone is predominantly used as solar filter in the UVA range (e.g. 320-380) and it is first chemical UVA filter that was approved by the FDA in 1988.

Metal complexes of β-diketones, e.g. avobenzone (Fig.1), are produced by mechanochemical reaction of at least one β-diketone and/or at least one polyphenol with at least one metal alkoxide according to Liliana's pending patents.[1]

Lili believes that these new polymeric complexes of avobenzone can overcome the safety issues of avobenzone in the USA regulation which is now under scrutiny with magnifying glasses. Since these new compounds based on avobenzone are bigger in the structure in comparison with the avobenzone alone and can be used as colored hydrophobic coating, probably, these novel compounds will be not able to enter to the blood stream and the risk of damage to humans and to the environment would be decreased.

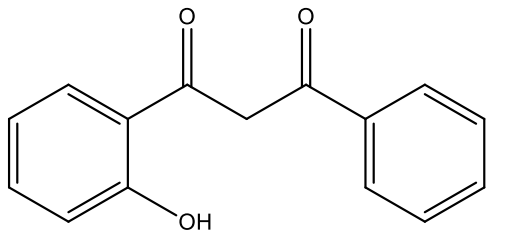
Fig. 2: Yellow avobenzone polymeric complex in a sunny day

Introduction

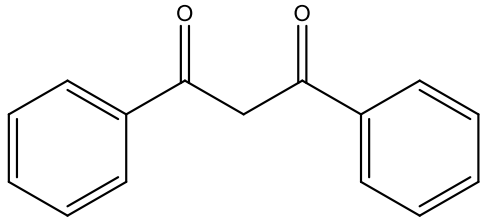
In lili's opinion many broad spectrum sunscreens do not protect against visible light nor are they suitable for dark-skinned people. Many cosmetic formulations contain colorants/mineral UVfilters, such as titanium oxide and/or zinc oxide and/or iron oxides, to match the color of the skin and/or to cover the whole UV range and therefore the stabilization of these formulations commonly is challenging as Liliana explained in her pending patents[1].

Today, lili would like to present to you one of her pigments/dyes based on one of the most used chemical filter in the market such as avobenzone—a β-diketone (see Fig. 1) and/or their derivatives (e.g., see Fig 3) with at least one metal alkoxide by mechanochemistry according to Liliana's pending patents[1] and to show that these complexes can be used as a UV filter without other ingredients or with less ingredients in the formulation.

Avobenzone is a white to pale yellow powder (Fig. 4, left) with a slight aromatic odor that can be found almost in every cosmetic product since it protects no only the skin but the product itself against UV rays. Avobenzone has a structure that changes/moves depending of the solvent or the environmental condition and therefore it is very unstable. Thus, the strong confinement of the avobenzone molecule by using my innovations will generate a more stable macromolecular structure.



1-(2-hydroxyphenyl)-3-phenyl-1,3-propanedione



1.3-diphenyl-1,3-propanedione

Fig.3: Chemical structure of some dibenzoyl derivatives

Hundreds of studies concerning the stability of avobenzone in the formulation have been or are still performed. In brief, the solutions are the combination of avobenzone with other UV filters, polymers, photo-stabilizers and so on. Nevertheless, lili's way of enhancing the stability of many compounds by mechanochemical complexation with metal alkoxide by green chemistry/cosmetics has been unheard of. Please see Liliana's pending patents to know the other strategies used to increase stabilization of many compounds that are markedly different from my approach.

Lili believes that so far solutions have been worse than the problem, since it is well known that many filters in the formulation increment the risk of destabilization and the production of possible toxics o allergens. Moreover, the use of excipients, preservatives and aromas creates another possible inset of allergies or destabilization (see lili's post on 27 September 2017 about avobenzone[2]).

Thus, it is common to find more than one filter in a formulation, and then the chance of producing allergic reactions is increased.

Here Lili would like to show that her avobenzone titanium complex is stable and has enhanced filter properties in comparison with avobenzone alone. Furthermore this new complex can act as a physical and chemical absorber/filter since titanium is present in the structure—any other appropriate metal such as zinc can be used as a source of metal from the metal alkoxide.

Results and Discussion

The titanium complex of avobenzone has an astonishing yellow color that are very stable in several solvents (Fig 4 (right) and 6 (right).

Lili's cosmetic formulations comprising the metal complexes of her invention are also very stable against light, storage and solvents, among others.

The supramolecular and/or polymeric structure of this novel avobenzone metal complex is produced by a self and/or forced assembly by the mechanochemical process according to my pending patents. Since the

Fig.4: Lili's new material based on avobenzone. Avobenzone is on the left and my novel complex is on the right. The color is more spectacular if you see directly in a sunny day. Lili's iphone does not reveal the

structure of my metal avobenzone complex is bigger than the neat avobenzone (proof thereof is the change in color see Fig. 4 and 6), there is less chance of this novel avobenzone complex being absorbed by the skin. In addition, its water repellent properties are beneficial for water sports activities.

No other kind of UV filter is needed; neither physical nor chemical filter is necessary.

Suffering from sun allergy myself, I can assure that my avobenzone complexes protect me from the sun in my own formulations and do not cause me allergy or worsen my existent allergy.

Lili can conveniently design the appropriate color (i.e., the structure) of my complex by using the processes according to Liliana's pending patents.

Lili's new colored pigment/dye based on the simple dibenzoylmethane (or its derivatives)—neither protecting groups nor leaving groups nor directing groups nor any other working groups are intentionally created or designed—are very stable to light, storage, temperature, to solvent e.g. water. Its water repellent properties makes lili's new complexes very apt to be uses as a sunscreen whenever people are in contact with water. The way to produce this new yellow pigment/dye

Fig. 5: Lili's new metal complex of avobenzone showing water repellence properties when applied directly onto lili's keratinous tissue.

is very simple, rapid and environment-friendly, since no toxic organic or aqueous solvents are added and no waste or (toxic) byproducts are produced. The scale-up is also ready. Just imagine that hundreds of tons of avobenzone that many companies are producing can be converted to a gorgeous yellow pigment/dye in only a few minutes with several applications, for instance, for replacing many toxic yellow dyes containing toxic metals such as lead, chromium, cadmium, arsenic or tin.

In addition, this new avobenzone metal complex can be used as a dye or pigment to paint people's creations in different subtracts.

Conclusions

Lili's metal complexes can be used as a UV filter. Moreover they can be used in formulations for every one since with the appropriated designed of the complexes according to my pending patents all colors of the rainbow can be produced. With subtle changes in the production or the formulation of this complex the color can be changed according to the color of the skin or to people's favorite color. If another metal (or no metal) alkoxide is used to perform the mechanochemical

reaction with avobenzone, different materials can be obtained with a diversity of colors. The sustainable product and production and the enhanced properties, such as solubility and color make my novel compounds very apt to be used as UV filter.

Fig.6: Avobenzone in the left and lili's new material based on avobenzone in the right

Outlook

Since avobenzone (sunscreens are considered drugs in U.S) is undergoing scrutiny by FDA-U.S. Food and Drug Administration[3] and is not "generally recognized as safe and effective"—or GRASE—for use in sunscreens because additional data needed, the complexation to form a stable pigment from it could help to overcome instability or allergy issues. Moreover many chemical sunscreens including avobenzone are currently banned from sale and to be used in many places in the world like Hawai. Recently, Jan. 1 2023, the center of biological diversity of Hawai banned the sale of sunscreens containing octocrylene and avobenzone.[4] They also make a petition to FDA to a national ban of coral-killing chemical in sunscreens. The process to produce metal avobenzone complexes deserves some attention, as it is well known that complexation reduce the toxicity of many compounds and it is recognized as a strategy to reduce safety issues such as in the case of toxic azo dyes. Big companies can make studies without hesitation regarding toxicity to humans and the environment of lili's new complexes. The use of only physical sunscreens such as titanium oxide and zinc oxide is not the optimal way since they do not cover the whole UV and some of the visible spectrum. Thus, safe and efficient chemical sunscreens are needed.

Lili believes that her portfolio of innovations on **doctora liliana cosmetics** regarding new polymeric solar filters can contribute in a positive way to the pollution caused by the conventional chemical filters without diminishing their function as protecting our skin from the sun.

"The less, the better" is lili's motto.

Let's go dance with Shakira

"Te estimo
Amarillo, me tienes en los bolsillos
Morado, ya me olvidé del pasado
En rojo, por que me sangran los ojos de llorarte
Cuando no estás a mi lado"

By Shakira

[1] **WO2021121647** - Metal complexes of macrocycles and/or isoprenoids and/or linear tetrapyrroles by mechanochemistry (grinding or milling), preparation method thereof, sunscreen/concealer/uv absorber thereof, self-assembled coating material thereof, superamphiphilic material or surfaces thereof, hair dyeing thereof and other uses thereof. **Priority Data** 18.12.2019
WO2019238261 - Metal complexes of β-diketones and/or polyphenols by green chemistry, preparation method thereof, sunscreen thereof, skin or hair tone concealer thereof, hair dyeing thereof and other uses thereof. **Priority Data**: 15.06.2018

[2] https://doctoralilianacosmetics.wordpress.com/2017/01/27/butyl-methoxy-dibenzoylmethaneavobenzona-acicalandose-con-el-malhechor/

[3] https://www.fda.gov/drugs/news-events-human-drugs/update-sunscreen-requirements-deemed-final-order-and-proposed-order;
https://dps-admin.fda.gov/omuf/omuf/sites/omuf/files/primary-documents/2022-09/Final%20Administrative%20Order%20OTC000006_M020-Sunscreen%20Drug%20Products%20for%20OTC%20Human%20Use.pdf

[4] https://biologicaldiversity.org/w/news/press-releases/hawaii-senate-bill-bans-harmful-sunscreen-chemicals-2021-03-09/

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