

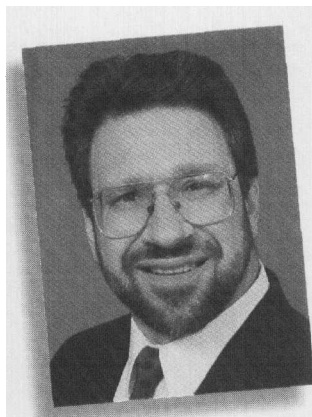
kosmetikos*

By Steve Herman

QUANTUM COSMETICS

"That all sounds good, but do we really want to use quantum mechanics?"

It is accepted wisdom that a cosmetic scientist needs a thorough background in chemistry. Familiarity with the anatomy and physiology of hair and skin, microbiology and a number of other disciplines are necessary for the Compleat Formulator. But what about quantum mechanics? It may not be the topic that initially pops to mind as we ponder the nuances of personal care. Yet there are aspects of cosmetic technology that are only explicable by evoking those tiny friends from physics class, the quanta.



At the turn of the century—the last turn, that is—key aspects of the “common sense” classical view of physics yielded successively to relativity theory, then quantum mechanics. The behavior of matter at the atomic scale was found to exhibit strange properties, one of which was an equivalence of waves and particles. Another was the discrete nature of energy. Energy

comes not in a continuous range of values but in discrete units dubbed “quanta.”

A model of the atom developed by Niels Bohr in 1913 took into account some non-classical discoveries. It consisted of a positive nucleus composed of protons and neutrons, surrounded by orbiting negative electrons. In classical physics, the atom would instantly self-destruct as the electron plunged toward the nucleus. Bohr postulated the presence of stable orbits which do not radiate. The theory was modified in 1924 by Sommerfeld, incorporating the wave nature of particles to explain the existence of the stable orbits.

A more abstract model of the atom pic-

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*Greek kosmEtikos, skilled in adornment or decorating.

tures the electrons as a cloud of negative charge centered in the location of the orbit. Aromatic molecules such as benzene have areas of delocalized shared electrons rather than individual electrons associated with single nuclei.

Fortunately, the only mathematics needed to understand the quantum phenomena of light interacting with atoms is contained in one tiny relationship:

$$E=h\nu \quad \text{where } E \text{ is the energy, } \nu \text{ is frequency, } h \text{ is Planck's Constant.}$$

Since the electrons can only occupy discrete orbitals, the only allowed energy differences are those connecting any two states (Figure 1). Using Planck's relationship, we see that the frequency of incoming radiation determines the jumps in energy possible in a molecule. Similarly, a molecule in an excited state can only lose energy in specific units.

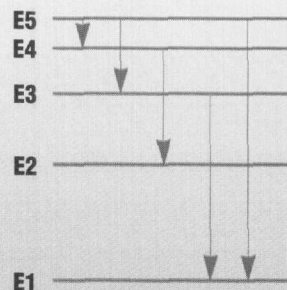
Visible light is part of the electromagnetic spectrum (Figure 2), which extends from gamma-rays to radio waves. We need only look at the region around the visual area, which represents most of the radiation the earth receives from the sun. The UV and visible areas both result in outer electron transitions. By contrast, x-rays cause inner electron transitions, and radio waves result in nuclear spin flips.

Light, the radiation our eyes process, has color. Let's look at a colorful molecule (Figure 3), a vibrant magenta. The structure has two benzene

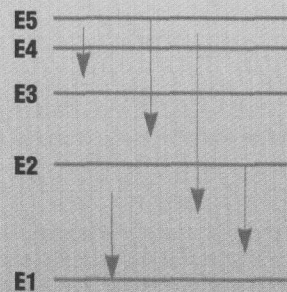
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Figure 1

ALLOWED TRANSITIONS



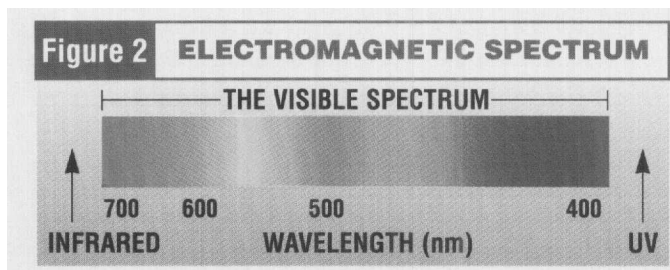
FORBIDDEN TRANSITIONS



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rings, another ring with two double bonds, and enough conjugation to sink a ship. There are two possible structures which have almost equal energies, and the electrons can flip



from one form to the other. Since there are so many electrons involved in the cloud, the amplitude of the flipping is lower than for benzene by itself. Benzene absorbs radiation, but at 200nm it is not detectable by humans. In our colored molecule, the difference in energy between the two states is equal to the energy of a photon in the optical region.

Thus, it has very strong absorbency at one frequency, and is perceived as brightly colored. We don't see the color which is absorbed but the complementary color. If red is removed, blue-green results.

The rate of change between states is closely related to the exact structure of the molecule, so slight changes can effect the color significantly. For example, replacing two hydrogens with methyl groups yields melachite green. Introducing small asymmetries also results in color modification.

A major group of colors, the azo dyes, are characterized by the presence of the $-N=N-$ group. The delocalized electrons contribute to resonance. The azo structure is one of a group of configurations called chromophores, all of which promote the ability to absorb radiation. Some other examples are $-C=N-$, $-C=O-$, and $-NO_2$.

The importance of sunscreens has been well established as a critical preventative measure in the war on skin cancer. There are two general types of sunscreens, physical blocks

like TiO_2 , and chemical blocks, which work by quantum mechanics!

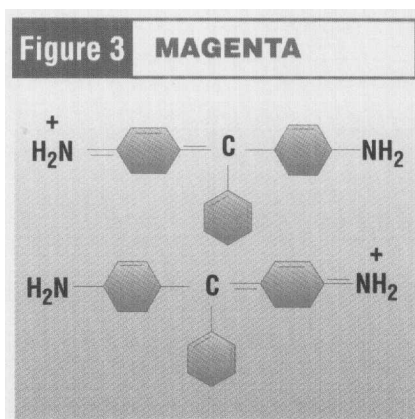
The UV light, which is particularly damaging, has a precise energy associated with its wavelength. The sunscreen must be capable of absorbing this exact energy and converting it into a harmless form. The loose clouds of conjugated electrons make this possible.

Where does the energy go when the UV is absorbed? The electrons are placed in a higher energy state. This can create an increase in temperature, so skin can feel warmer when using a sunscreen. If light is emitted in the return to ground state, fluorescence results, so sunbathers can glow. Returning to our dyes, a chemical change can occur, resulting in fading.

A thorough account of the exact mechanism of sunscreen activity was provided by Shaath², and interested readers are urged to start with him. In brief, the organic sunscreen takes harmful radiation (250-

350nm) and releases the energy in longer wavelength forms as it returns to the ground state. The more resonance present, the more effective the sunscreen chemical.

Without probing too deeply into the world of theoretical physics, we see that a number of phenomena significant in personal care can only be understood when quantum principles are considered. It is not necessary to grapple with the full mathematical glory of the quanta. Simply to remember that waves, specifically visible light and UV, have associated energy, and that appropriate molecules can absorb and modify the energy packets. ■



References:

- For an overview with links of quantum mechanics on the web, see <http://www-theory.chem.washington.edu/~trsted/quantum/quantum.html>
- A useful overview of the theory of dyes is on <http://members.pgonline.com/~bryand/dyes.htm>
1. <http://wilson.ucsd.edu/education/qm/14.WhyQuantum2.jpeg>
 2. Shaath, Nadim A.. On the theory of ultraviolet absorption by sunscreen chemicals. *JSCC*, Vol. 38, No. 3, May/June 1987.