Supplementary Appendix I

Color is caused by selective absorption of a given illuminating light when it passes through a transparent substance or when it is diffusely reflected from the surface of non-transparent or powder material. Illuminating light often consists of a mixture of different monochromatic radiation occurring in the visible range (Supplementary Fig. 2) in such proportions that the human eye perceives colorless white light. Upon passing through a transparent substance, different wavelength radiation can be selectively absorbed or not and in varous amounts. This selective absorption of radiation in the visible (Vis) region of the electromagnetic spectrum, which is located between the shorter wavelength ultraviolet (UV) and longer wavelength infrared (NIR) regions, results in color.

A colorimetric system be analyzed based on the fact that any color can be reproduced through the mixing of various combinations of other colors[1]. The mixing process can be demonstrated, for example, by projecting various combinations of colored light beams onto the same area of a diffuse reflecting white screen. Here, it can be shown that different combinations of light and their amounts can give rise to the same resultant color. This mixing behavior can also be shown through the blending of various combinations and amounts of colored pigments to produce the same color of paint, for example. The way humans perceive color is a subjective psychological phenomenon, because the precise spectral composition of the mixing colors does not play a role.

[1]We omit any discussion of other types of colorimetric systems, for example, those, based on visual comparison of a sample with color standards (e.g. the Munsel color system – Judd and Wyszecki 1963).

The number of combinations of different colors that can mix to produce a certain given color is infinite. This fact is described by Grassman's law, which governs the optical composition of

color. It gives the minimal number of colors necessary to reproduce any existing color through mixing and is equal to three and is given by:

$$C_0 = aC_1 + bC_2 + cC_3, \qquad (1),$$

where C_1, C_2 and C_3 are the so-called independent colors. No independent color can be obtained through the mixing of the other two. For instance, they may be red, green and blue. Grassman's law has no physical meaning because it describes the purely psychological aspects of visual color perception. Following (1), any color, C_0, can be expressed three dimensionally and may be represented by the sum of three independent color vectors C_1, C_2 and C_3, whose magnitudes can be different (defined by the coefficients a, b and c). C_1, C_2 and C_3 are called the primary colors or the color stimulus for a given colorimetric system.

The Commission Internationale de l'Eclairage (CIE) in 1931 adopted the first three-stimulus colorimetric system termed *RGB*. The primary colors were red, green and blue having monochromatic wavelengths of 700.0 (R), 546.1 (G) and 435.8 (B) nm, respectively. One has $F = rR + gG + bB$, whereby any color, F, can be made through a mixture of R, G and B taken in the amounts r, g and b. A more convenient representation, where the color stimuli are only additive in nature, and do not necessarily involve subtraction as in the case of some colors of the *RGB* system, is given by the CIE colorimetric system XYZ. Here, the primary colors X, Y and Z are hypothetical and they mix to produce any possible resultant color. This system arises through a mathematical transformation of the *RGB* system. It is based on the same principles, namely, that any color can be specified by the quantities of three different illuminations. The main difference of the XYZ system from the *RGB* system is that the colors of its primary "illuminations" X, Y and Z exist only as colorimetric equations. The colors themselves are not reproduced. The XYZ description forms the basis of all modern colorimetric systems.

The primary colors X, Y and Z are represented by three orthogonal unit vectors and all possible colors, obtained through their mixing, are contained within a closed color-space volume. A color vector, F, can be written as:

$$F = x'X + y'Y + z'X \quad (2),$$

where x′, y′ and z′ are the coefficients that define the relative amounts of X, Y and Z. Equation (2) describes color quantitatively. For a description of color, the values of chromaticity and brightness are used. They express the qualitative and quantitative characteristics of color, respectively. Chromaticity is defined by the coordinates:

$$x = \frac{x'}{x' + y' + z'},\ y = \frac{y'}{x' + y' + z'} \text{ and } z = \frac{z'}{x' + y' + z'} \quad (3)$$

and, because $x + y + z \equiv 1$, two coordinates suffice for its determination. Usually, x and y are taken.

The value of brightness is described by y'. It characterizes the visual perception of light transmittance or reflectance (in the case of non-transparent diffuse reflection) of a substance. The orthogonal chromaticity x-y diagram (Supplementary Fig. 3) is typically used for the illustration of color. It is a two-dimensional projection from the (1,1,1) section in X-Y-Z space, where the orientation of the main color axes is taken in a such way that the X + Y + Z = 1 plane gives a right triangle. Here, all real colors lie in an area bounded by a curve that defines the most saturated spectral colors of monochromatic illuminations in the visible range from 380 to 700 nm and a straight line that connects the ends of this curve. This latter line is the locus of the most saturated purple colors. Point C is the locus of the standard white illuminator, C, representing dispersed North sky daylight.

For a description of chromaticity, the dominant wavelength, λ_k, and the color saturation value, p_c, are typically used. For example, for the color F_1 having the coordinates $x_1 = 0.32$ and $y_1 = 0.6$, λ_k is about 554 nm and $p_c = CF_1/C\lambda_k \cong 0.81$ (Supplementary Fig. 3). λ_k describes the dominant color, which is yellowish-green in this case. p_c gives the amount of spectral color, λ_k (dominant wavelength), which should be mixed with the color white, C, to reproduce the color F_1 having the coordinates x_1 and y_1. In comparison, the color of F_2, which does not have a dominant wavelength, is purple (i.e., a mixture of red and blue light). Its saturation value, p_c, is given, once again, by $p_c = CF_2/CP \cong 0.75$. Instead of using λ_k, the value of the supplementary spectral color $\lambda_k' \sim 502$ nm is taken. All colors, which lay within the triangle defined by 380 nm, point C, and 700 nm (Supplementary Fig. 3), have an infinite number of purple colors that do not have spectral analogues. Therefore, their λ_k' and p_c values should be determined as done for color F_2. For further aspects behind the colorimetric system XYZ, the reader is referred to Judd and Wyszecki (1975).