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Molar extinction coefficients and the photon absorption efficiency of dental photoinitiators and light curing units

Miguel G. Neumann[a,*], Walter G. Miranda Jr.[b], Carla C. Schmitt[a], Frederick A. Rueggeberg[c], Ivo C. Correa[b]

[a]*Instituto de Química de São Carlos, Universidade de São Paulo, Caixa Postal 780, 13560-970 São Carlos SP, Brazil*
[b]*Faculdade de Odontologia, Universidade de São Paulo, Brazil*
[c]*Medical College of Georgia, School of Dentistry, Augusta, USA*

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Quartz-tungsten-halogen (QTH);
Molar extinction coefficient;
Photon absorption

Summary *Objectives*. The light absorption of dental photoinitiators should correlate with the spectral emission profiles of dental light curing units compared on an equivalent basis. Spectral data of dental photoinitiators and light curing units can be used to define the photon absorption efficiency (PAE) obtained by integrating the product of the absorption and emission spectra in terms of photons. This parameter can be used to identify the best performance for photochemical process with specific photoinitiators.

Methods. The efficiency of two LED and one QTH lamps were tested comparing their performances with the photoinitiators camphorquinone (CQ); phenylpropanedione (PPD); monoacylphosphine oxide (Lucirin TPO); and bisacylphosphine oxide (Irgacure 819). Absorption and emission spectra of the photoinitiators and the LED (Ultrablue I and Ultrablue IS) and QTH (Optilux 401) LCUs were determined in the 360–550 nm range.

Results. CQ exhibited an absorption centered in the blue region and, although the maxima of PPD, MAPO, and BAPO were in the UV-A region, their absorption extended to the visible region. Power output maxima of the LCUs were at 467 (Ultrablue I), 454 (Ultrablue IS) and 493 nm (Optilux 401), and the total power densities were 170±1, 470±4 and 444±4 mW/cm^2, respectively.

Significance. The use of the PAE allows a prediction of the most efficient photoinitiator/LCU systems. For similar photoinitiator concentrations, Lucirin and CQ are most efficiently photoinitiated by the QTH unit, whereas the high-power LED device is more efficient for Irgacure. PPD is photoactivated similarly by both LCUs.
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Introduction

The resin matrix has an important influence on the chemical and physical properties of light cured

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[*] Corresponding author. Tel.: +55 46 3373 9940; fax: +55 46 3373 9952.
E-mail address: neumann@iqsc.usp.br (M.G. Neumann).

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resins. In the past four decades, no fundamental change occurred in the dimethacrylate formulations based on BisGMA.[1,2] The organic formulations also include photoinitiation systems that absorb light and take the molecules to excited states. From there, radicals or other initiating species start the conversion of the oligomer blend to a polymeric crosslinked network.[2,3]

Absorption requirements of dental photoinitiators should correlate with the spectral emission profiles of dental light curing units (LCU). The visible light photosensitizer camphorquinone (CQ) is widely used in dental resin and adhesive formulations.[2,4] CQ is a solid yellow compound with an unbleachable chromophore group, so that large amounts of CQ in resin formulations will lead to an undesirable yellowing, affecting the final aesthetic appearance of the cured material.[5-9] After light absorption between 400–500 nm (maximum at 470 nm) CQ is promoted to an excited triplet state that interacts with an electron- or proton donor molecule, like a tertiary amine, to generate free radicals.[2-4]

Since the light absorption process of the photoinitiators or photosensitizers is fundamental to improve the photochemical reaction efficiency, it is important to select compounds with absorption spectra that overlap with the emission spectra of the irradiation sources. Recently, manufacturers included different photoinitiators in the organic matrix to act alone, or synergistically, with CQ.[8] Compounds derived from acylphosphine oxides and α-diketones are used in adhesives and composite resins formulations to improve the polymerization kinetics and lessen the photoyellowing effects.[7,8,10,11] Unlike CQ, the absorption peak of these compounds is mainly in the near UV region (UV-A) and extends slightly into the visible region.[8,12,13] The generation of free radicals from these compounds will not be very efficient when using light-emitting diode (LED) sources, which do not have high emission intensity in this region, but probably might be efficient when the broad band emission of a quartz tungsten-halogen (QTH) light-curing unit is used.

The probability of light absorption by a molecule depends on its extinction coefficient (ε_λ),[12] and on the number of photons available that can be absorbed. Large values of ε indicate a high probability of absorption at a given wavelength, leading to large quantum yields of the initiating species and, consequently, improving the polymerization kinetics and overall conversion.[12,14] The efficiency of various visible light LCUs used with CQ-containing formulations was evaluated by Cook,[15] showing qualitatively the need of a good overlap between the emission of the lamps and the absorption spectrum of CQ. More recently, Stahl et al.[16] and Teshima et al.,[17] analyzed several LCU/photoinitiator systems by a method similar to that described in this work, but based on the energy output of the light sources, instead of the number of photons.

The aim of this study is to determine the molar extinction coefficient of four photoinitiators and the power density profiles of LED and QTH light curing units. The product of both spectra in terms of photons was integrated to calculate the photon absorption efficiency (PAE) of each LCU/photoinitiator pair, that can be used to evaluate the conditions for improving the photochemical process when using those photoinitiators.

Methods and materials

Absorption spectrophotometric analysis

The photoinitiators monoacylphosphine oxide or MAPO (Lucirin TPO, BASF), bisacylphosphine oxide or BAPO (Irgacure 819, Ciba-Geigy), phenylpropanedione (PPD, Aldrich) and camphorquinone (CQ, Aldrich) were used as received (Fig. 1). The solvent used was methyl methacrylate (MMA 99% HPLC, Fluka).

Solutions of the photoinitiators in methyl methacrylate were prepared taking into account the solubility of these compounds and are shown in Table 1. No hints of reaction of the solvent were observed after the spectroscopic measurements.

Absorption spectra were determined in the 200-600 nm range using a UV-Vis spectrophotometer (Hitachi U-2000), although only the visible and near UV range was of interest (360–550 nm), as this range reflects the emission of most QTH based curing units. The spectra were taken using a 1.0 cm pathlength quartz-cell. Absorption spectra were recorded for each photoinitiator and the ε_λ were calculated from the absorbance values in the original solutions, using the Beer-Lambert law

$$\mathrm{Abs}_\lambda = \varepsilon_{\mathrm{L/mol\ cm}}[c_{\mathrm{mol/L}}]L_{\mathrm{cm}} \qquad (1)$$

where Abs is the absorbance at each wavelength, ε is the molar extinction coefficient, $[c]$ is the concentration of the photoinitiator in the solution and L is the optical pathlength.

Emission spectrophotometric analysis

The LCUs used in this study were: (1) Optilux 401 (OPT, Demetron Inc., Danbury, MA, USA) a QTH unit

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