TRUE ABSORPTION CAPACITY OF CERTAIN
PHARMACEUTICAL PREPARATIONS

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The absorption of radiant energy by drugs (caffeine and sulfadimezene) is analyzed. The most effective absorption bands are determined.

For the heat treatment of pharmaceutical preparations it is necessary to know the characteristics of the radiation source (specifically, the spectral energy density) and also the absorptivity of specimens.

From a knowledge of the spectral density distribution of energy emitted by the source, together with the absorptivity as a function of the wavelength $A(\lambda)$ or of the wave number $A(\nu)$, it is possible to determine the ranges of the spectrum where the absorption of radiant energy is maximum and, consequently, the heat treatment will be most effective.

The energy absorbed by a material within the range of the spectrum from λ_1 to λ_2 or from ν_1 to ν_2 is

defined as $\int_{\lambda_1}^{\lambda_2} u(\lambda)A(\lambda)d\lambda$ or $\int_{\nu_1}^{\nu_2} u(\nu)A(\nu)d\nu$; $u(\lambda)$ and $u(\nu)$ denote the spectral density of radiant energy in

terms of wavelengths or wave numbers, respectively.

An analysis intended to find the most effective absorption bands has been made for two chemical drugs in a disperse state with very distinct physicochemical properties: sulfadimezene and caffeine. 2-(n-Aminobenzosulfamido)-4,6 dimethylpyridine (sulfadimezene) is a white, slightly yellowish, powder. Its melting point is within 197-200°C [2]. 1,3,7-Trimethylxanthine (caffeine) is a white silky substance in the form of acicular crystals or a crystalline powder. Its melting point is within 234-237°C [2].

Because these substances melt at such low temperatures, it becomes necessary to use a low-temperature radiation source. The subsequent calculations apply to a radiator at T = 450°C, the energy density of which is described by the Planck function $u(\nu, T)$.

The wave number corresponding to the maximum of this $u(\nu, T)$ function is

$$\nu_{max} = 1.9610T \text{ cm}^{-1} \tag{1}$$

and for our radiator this amounts to 882.45 cm^{-1}.

We will also determine the wave numbers corresponding to half the maximum radiant energy density, i.e., $(1/2)u(\nu, T)_{max}$ on both sides of ν_{max}:

$$\nu_{1/2}^{(1)} = 0.8045T \text{ cm}^{-1}, \ \nu_{1/2}^{(2)} = 3.7612T \text{ cm}^{-1}. \tag{2}$$

The quantity

$$\nu_{1/2}^{(2)} - \nu_{1/2}^{(1)} = 2.9567T \text{ cm}^{-1} \tag{3}$$

may be treated as the equilibrium radiation band of the spectrum.

It has been noted in [1] that the major part (75.4%) of the total energy is emitted over the $\nu_{1/2}^{(1)}$ to $\nu_{1/2}^{(2)}$ band (30.4% from $\nu_{1/2}^{(1)}$ to ν_{max} and 45% from ν_{max} to $\nu_{1/2}^{(2)}$). Only 5% is emitted at frequencies below $\nu_{1/2}^{(1)}$
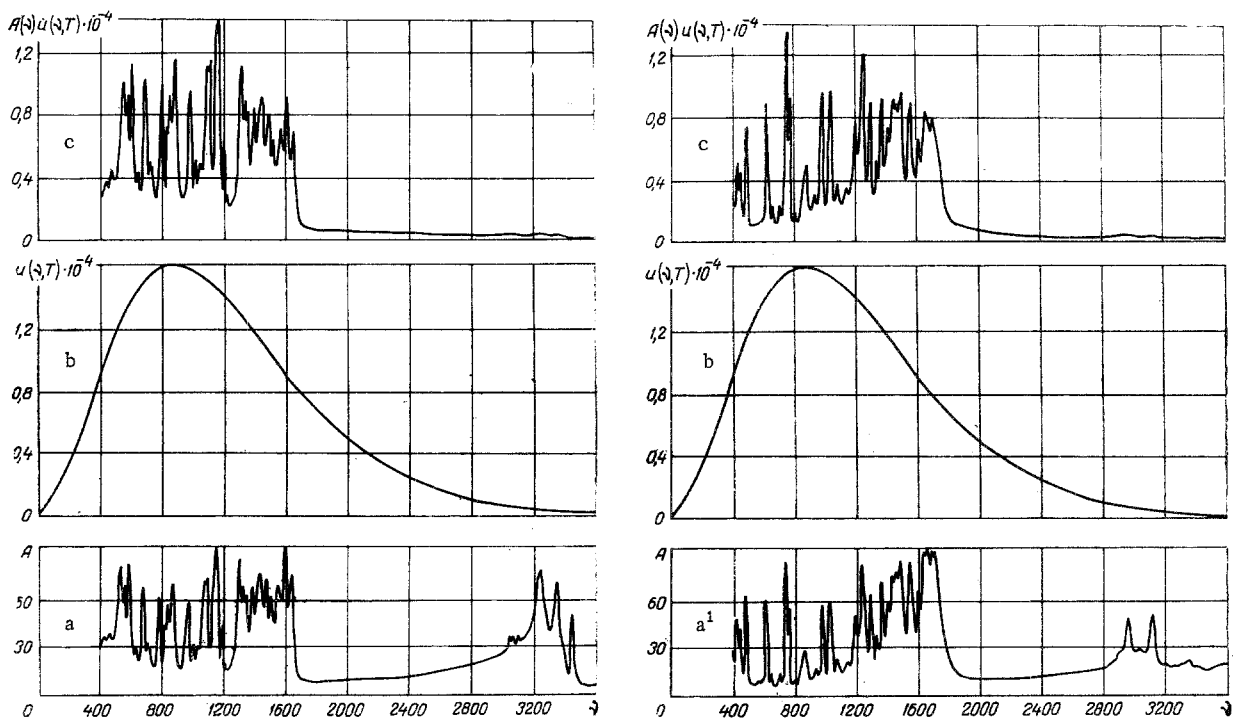
Fig. 1. Infrared spectrum of sulfadimezene (a) and caffeine (a^1), spectral density of equilibrium radiation $u(\nu, T)$ ($W/cm^{-2} \cdot cm$) at $T = 450°K$ (b), and curve of effective absorption $u(\nu, T)A(\nu)$ ($W/cm^{-2} \cdot cm$) (c). A, %.

and 19.6% is emitted at frequencies above $\nu_{1/2}^{(2)}$.

For our particular radiator these wave numbers are:

$$\nu_{1/2}^{(1)} = 362.025 \text{ cm}^{-1};$$

$$\nu_{1/2}^{(2)} = 1692.54 \text{ cm}^{-1};$$

$$\nu_{1/2}^{(2)} - \nu_{1/2}^{(1)} = 1330.515 \text{ cm}^{-1},$$

i.e., 75.4% of the emitted energy is contained within the 362.025-1692.54 cm^{-1} band.

As the criterion of the absorption characteristics of these two substrates we have chosen their infrared absorption spectra. These spectra were recorded with a UR-20 two-beam spectrophotometer. The specimens had been prepared by molding with KBr [3, 4].

As can be seen in Fig. 1, the absorption bands of sulfadimezene are 400-1700 cm^{-1} and 3000-3500 cm^{-1}, while those of caffeine are 400-1800 cm^{-1} and 2900-3200 cm^{-1}, i.e., the absorption bands of the two substances nearly overlap: 400-1800 cm^{-1} and 2900-3500 cm^{-1}. Further calculations were made to determine the bands of maximum absorption. For this purpose, we analyzed the variation of the product $u(\nu, T)A(\nu)$ within the range 400-5000 cm^{-1}.

The range of low wave numbers (< 400 cm^{-1}) is not considered, since it has not been possible to obtain data on absorption within this range, but it may be assumed that this absorption is not an appreciable fraction of the total absorption, since the energy emitted in this range amounts to only 7% of the total emitted energy.

Figure 1 shows the infrared absorption spectrum, the spectral density of equilibrium radiation [$u(\nu, T)$], and the curves of effective absorption [$u(\nu, T)A(\nu)$] of sulfadimezene and caffeine.

The trend of the $u(\nu, T)A(\nu)$ curve within the 400-1800 cm^{-1} band is approximately the same as that of the $A(\nu)$ spectrum. This is logical because, the spectral energy distribution being a continuous function of the wave number, the emitted energy density is approximately $(1/2)u(\nu, T)_{max}$ even at the corners of the band, while the absorptivity inside this band varies much more.

As can be seen in Fig. 1c, almost all the absorbed radiation energy coming from the source is in the $400-1800$ cm^{-1} band. Between 1800 and 2900 cm^{-1} there are no absorption bands, even though the density of emitted energy is still not very low:

$$\frac{u(\nu=1800,\ T)}{u(\nu,\ T)_{max}}=0.432,\quad \frac{u(\nu=2900,\ T)}{u(\nu,\ T)_{max}}\approx 0.05,$$

and because of the small value of $A(\nu)$, there is no significant contribution here to the total absorbed energy to speak of. Within the $2900-3200$ cm^{-1} range (caffeine) and the $300-3500$ cm^{-1} range (sulfadimezene), on the contrary, there are absorption bands but the emitted energy density is low:

$$\frac{u(\nu=2900,\ T)}{u(\nu,\ T)_{max}}\approx 0.05,\quad \frac{u(\nu=3500,\ T)}{u(\nu,\ T)_{max}}\approx 0.01,$$

and the value of the product $u(\nu,\ T)A(\nu)$ is by one or two orders of magnitude lower than in the $\nu=400-1800$ cm^{-1} range.

The short-wave range ($3600-5000$ cm^{-1}), although not shown on the diagram, may be disregarded, because it contains no absorption bands and the emitted energy density is by 2 to 4 orders of magnitude lower than within the $400-1800$ cm^{-1} range.

Thus, almost all the energy emitted by the source is absorbed within the rather narrow $400-1800$ cm^{-1} band of the spectrum. It is important in the calculations to know not only $A(\nu)$ but also the mean absorptivity over a definite band of the spectrum:

$$A_{mean}=\frac{\int_{\nu_1}^{\nu_2} u(\nu,\ T)A(\nu)\,d\nu}{\int_{\nu_1}^{\nu_2} u(\nu,\ T)\,d\nu}. \tag{4}$$

Since in our tests infrared radiation is absorbed mainly within the $400-1800$ cm^{-1} band, the mean value here refers to this particular band. For sulfadimezene $A_{mean}=0.524$ and for caffeine $A_{mean}=0.424$.

The absorptivity of a material may change in the process of heat treatment. In order to take this possibility into consideration, we examined the absorption spectra of specimens heated to different temperatures. No significant changes in the absorption were observed: the radiation intensity had changed by 4-6% within the band peaks and by slightly more at the band corners. Thus, one may consider the absorptivity of a substance to remain constant during the heating process, until the aggregate state of the substance changes. It is to be noted that this discussion pertains to the proper absorptivity not including the effects of particle concentration, size, etc.

NOTATION

A	is the absorptivity;
λ	is the wavelength;
ν	is the wave number;
$u(\nu,\ T)$	is the spectral density of emitted energy;
T	is the temperature.

LITERATURE CITED

1. P. A. Apanasevich and V. S. Aizenshtadt, Tables of Energy and Photon Distributions in the Equilibrium Radiation Spectrum [in Russian], Izd. AN BSSR, Minsk (1961).
2. Government Pharmacopoeia [in Russian], Moscow (1968).
3. U. Schiedt and H. Reinwein, Zeitschr. Naturforschung, 7b, 270 (1952).
4. M. Stimson and M. O'Donnell, J. Am. Chem. Soc., 74, 1806 (1952).