Letter

Comment on the publication of transient spectra obtained using flash techniques†

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Transient absorption spectra obtained using techniques such as laser photolysis, conventional flash photolysis or pulse radiolysis are usually derived from the analysis of signal *versus* time profiles obtained at different wavelengths. In other words, they are derived from "point-by-point" measurements. However, a considerable fraction of the spectra published do not include the actual experimental points and provide only a rather poor description of the experimental conditions. Publishing the information in this manner takes up the same space as publishing spectra including the proper data and conditions, but in the former case the information is just about as useful as giving λ_{max} in the text.

Figure 1 illustrates the absorption spectrum of the phenanthrene triplet. Figure 1(a) shows only a continuous trace; it should be noted that this trace is simply the "artist's interpretation" of the original experimental data. In Fig. 1(b) the trace is the same, but the inclusion of the points clearly shows how much "artist's creativity" was required to obtain the continuous trace. The spectrum in Fig. 1(b) includes measurements at 16 different wavelengths obtained at 15 nm intervals in the region of interest and every 20 nm at $\lambda > 520$ nm. Intervals of this magnitude are common in experiments of this type.

The trace in Fig. 1(c), which is based on 63 measurements, is substantially different from that in Figs. 1(a) and 1(b); however, the experimental data are in full agreement with those of Fig. 1(b). Thus the importance of including experimental points should be self-evident. The following conditions were used in this experiment.

Phenanthrene (0.0016 M) in absolute ethanol (1 ml) was contained in a Suprasil cell with an optical path of 0.3 cm. Deaerated samples were excited at 27 °C with pulses (337.1 nm; about 8 ns; about 10 mJ) from a nitrogen laser. The rise time of the detection system was about 3 ns and the band-

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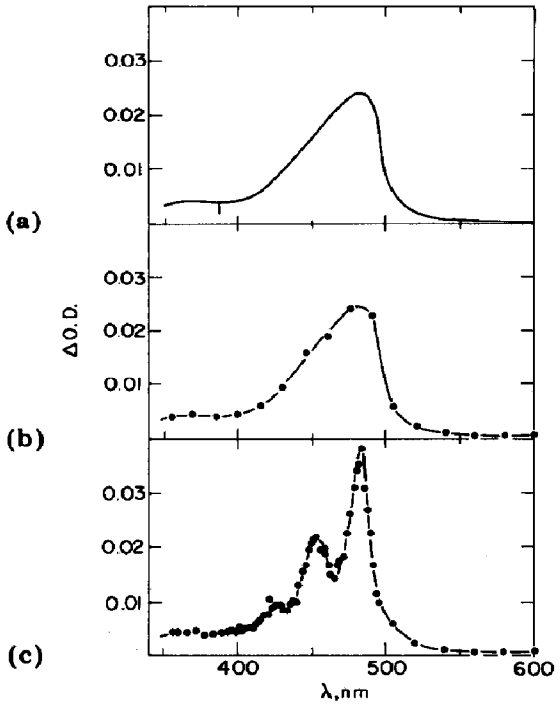

Fig. 1. Absorption spectra of triplet phenanthrene in absolute ethanol: (a) the continuous trace based on the experimental data given in (b); (c) spectra including measurements at 63 different wavelengths.

width was less than 1 nm. The spectrum shown was recorded by averaging the transient data starting 1.0 μs after the laser pulse (to avoid singlet absorptions) and during a time window of 1.0 μs. The instrument has been described elsewhere [1].

We believe that it would be quite useful to other colleagues working in the field, and to readers in general, if authors made a point of including the details of the experiments (as in the paragraph above) and the actual experimental points. In our view journals should reject spectra that do not conform to these criteria. Error bars may be desirable in some cases, although they are usually hard to estimate. If *all* the data are included their dispersion will give the reader a good idea of the magnitude of random errors.

1 J. C. Scaiano, *J. Am. Chem. Soc.*, *102* (1980) 7747.