

Preface

The *UV Spectra, Vapor Phase, 168- 330 nm* is intended for paying attention to the valuable quality of the ultraviolet (UV) spectrophotometry for scientific studies and as a measuring tool for numerous applications in every field, where classification, identification and quantification of compounds are required. Furthermore, the collection of the UV spectra vapor phase should satisfy the educational needs for courses on organic, analytical and physical chemistry as well as on applied physics. There are a number of advantages of being able to make measurements in the vapor phase rather than in the liquid phase. The spectra given are not influenced by any solvent effects and therefore very well defined and considerably more detailed. Furthermore, the wavelength range is not limited by the cut of wavelength of a solvent.

The *UV Spectra, Vapor Phase, 168- 330 nm* is a contribution to other handbooks of spectra as infrared (IR), nuclear magnetic resonance (NMR), mass (MS) and UV liquid phase and makes it possible for chemists and physicists dealing with research, education and practical work in industry and other laboratories to complete these handbooks. For most of the data in this collection of UV spectra vapor phase, the corresponding data for the compounds are found in the IR, NMR and MS spectra collections and can, consequently, be preferably used for completing and comparison.

Measurements of spectra presented in this book were made by means of a UV spectrophotometers constructed by Dr. Verner Lagesson. The optical configuration with the reverse optical bench was analogous to systems for HPLC photo diode array detectors. The whole light path was flushed with dry nitrogen (1 L/min) in order to prevent the light absorption due to water vapor and oxygen at wavelengths below 195 nm. The gas flow cell was made from an electrically conducting material and was temperature controlled. Deuterium lamp, 30 W (Hamamatsu), was placed in the lamp housing (Oriel Instruments). Quartz lenses focused the light beam between deuterium lamp - gas flow cell and gas flow cell – monochromator entrance slit. The Spectrograph, MS125 (Oriel Instruments) with focal length of 120 mm and a variable slit width was supplied with a 1200 l/mm holographic grating, blazed at 250 nm. The wavelength range could be varied by means of a micrometer screw influencing the angle of the grating. Throughout the recordings the wavelength range was set to be from about 165 nm to 330 nm. A photo diode array detector (Andor), with 1024 diodes 25.6 x 2.5 mm active area, collected the primary measuring data. These primary data were then imported to a Grams program (Thermo Galactic) for further treatment.

The instruments were calibrated regularly by means of the mercury emission line at 253.7 nm. This calibration was performed keeping the wavelength range linear in order to be able to make various calculations using the Grams program. The spectra of a number of identical reference compounds, taken from various laboratories in Sweden, were measured several times during sex years. **Fig. 1a** shows year to year variation in the spectral shapes of 4-nitroaniline in a normalized and overlaid mode. In order to amplify the details the absolute values of the first derivatives are also plotted in **Fig. 1b**.

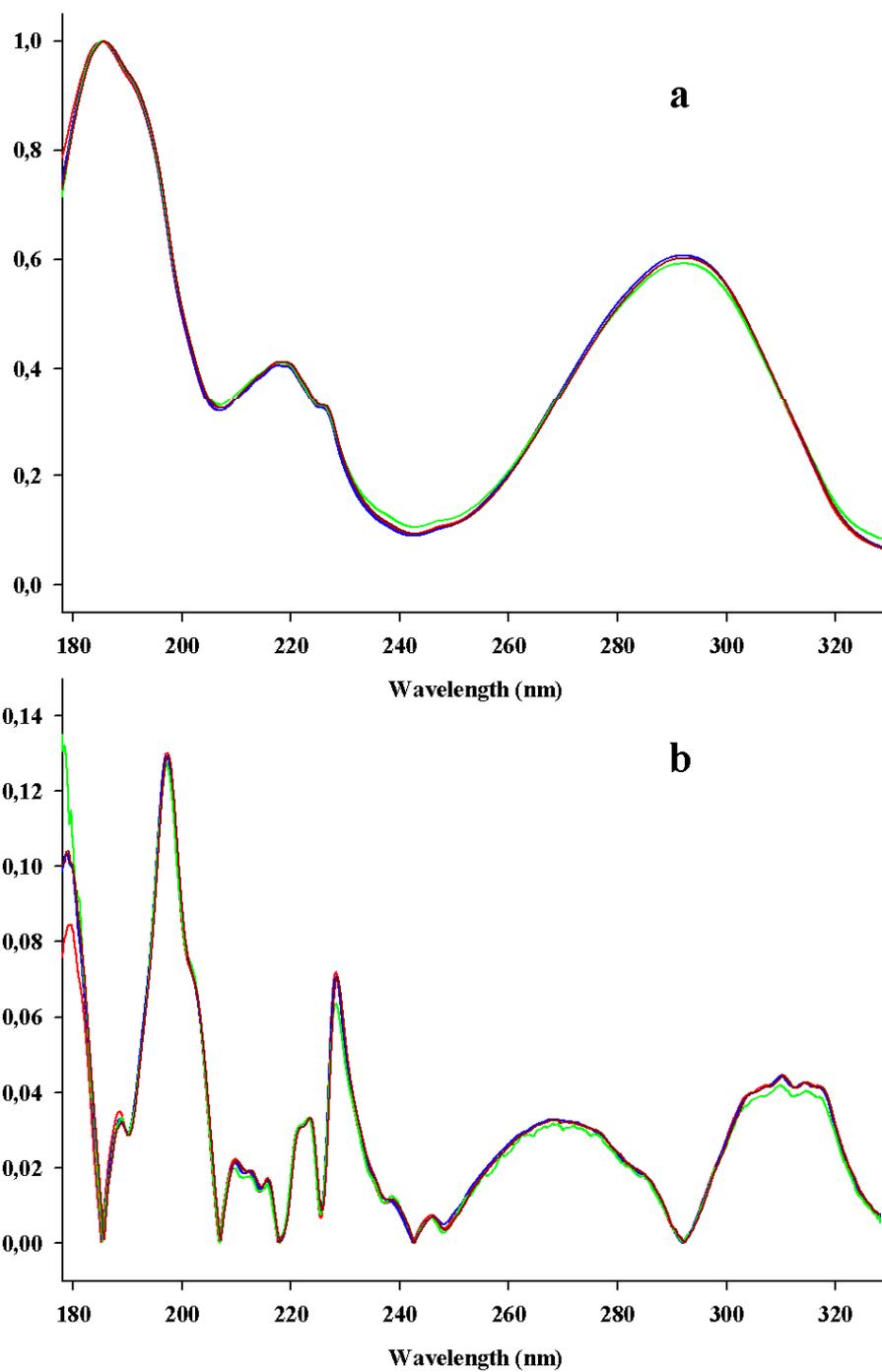


Fig. 1 a/ Overlaid normalized absorption spectra for 4-Nitroaniline recorded during a period of several years b/ first derivatives with absolute values for the same spectra as in a/

For the 1349 spectra presented in this collection, 70 % showed absorption maxima shorter than 190 nm. Besides being of general importance for sensitivity reason, the access to the low wavelength region also increases considerably the extent of spectral details. Furthermore, functional groups not being considered of interest for UV spectrophotometric studies (e.g. aldehydes, ketons, ethers and even alkanes) show their whole spectral information in this region.

Reference compounds were of various quality and from various sources. They were collected from chemistry departments at universities and research institutions in Sweden. The reference compounds were usually dissolved in either hexane or acetonitrile prior to injection. These solvents were selected, because of their low absorptivities at short wavelengths.

All spectra were recorded after a gas chromatographic (GC) separation. During the GC separation spectra were collected in 4 or 2 second intervals and the collected spectra were compensated for adjacent background spectra. The band width was 1.7 nm throughout the recordings, except for nitric oxide and sulphur dioxide, which were also recorded at a band width of 0.7 nm. The temperature of vapor in the light pipe varied somewhat depending on the boiling point of the compound analysed. Every measuring temperature is specified for each spectrum in this collection.

The 1349 spectra are presented on pages 1 - 484. Their position in the book, according to the table of contents, is made after their functional belongings, which follows, on the whole, the Aldrich's FT-IR collection. For each spectrum values for density, boiling or melting point, CAS number, FT-IR number, chemical formula and temperature of the vapors in the light pipe are given. For a number of compounds the CAS number has not been found. The FT-IR number refers to the "Aldrich Library of FT-IR Spectra Vapor Phase" Edition I, Volume 3, 1989. The spectra of compounds belonging to the same functional group are also depicted in the same figure in a normalized and overlaid mode. In this way 167 functional groups are recognized and shown on pages G-1 to G-167 in an alphabetic order. In the same manner 136 groups of isomers are shown on pages I-1 to I-68.

An artistic illustration introduces each main functional group section. The illustration contains one spectral curve with the wavelength scale and one created figure. They form together a picture of a scientific truth, concerning the measured appearance of a molecule, and of the pure imagination, which shows, how one can imagine the appearance. The existing conditions of the created figure is the nano horizon. Furthermore, the figure is connected with the spectral curve as its property, which is UV visible. The connection takes place at the absorption maximum as the main characterisation of the spectra. The human eye can not see the UV rainbow, therefore the visible rainbow is in the pictures. Each figure has also the chemical formula somewhere on its body showing man's understanding of the nature of a molecule.

Indexes in this book are arranged according to the spectra of the compounds in a functional group order with an alphabetical order under the subclasses. The overlaid spectra within the same functional group and the groups of overlaid spectra of isomers are approximately following the same functional group order as for the individual spectra. Also a CAS number index in an ascending order is given.

