SPECTRAL ATLAS of POLYCYCLIC AROMATIC COMPOUNDS Vol. 3

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including information an aquatic toxicity, occurrence and biological activity

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Preface

This volume is the 3rd in a series of comprehensive publications devoted to the molecular spectra and environmentally important properties of polycyclic aromatic compounds which constitute one of the most interesting classes of environmental carcinogens.

Since the first identification of dibenz(a,h)anthracene and later benzo(a)pyrene as chemical carcinogens in the 1930's, the number of publications devoted to this ubiquitously occurring group of compounds has increased constantly.

Therefore, this reference source for the spectral, physicochemical and environmental properties of polycyclic aromatic compounds should be a welcome addition to the previous volumes for scientists engaged in the investigation, characterisation and control of this hazardous class of pollutants.

As was the case with the preceding volume, this publication is the fruit of a close collaboration within the General Directorate for Science, Research and Development of the Commission of the European Communities between the Environment Institute of the Joint Research Centre Ispra, the Community Bureau of Reference and expert laboratories in the member states.

F. Geiss
Director of the Environment Institute
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1. Introduction

Polycyclic Aromatic Compounds (PAC) are an important class of carcinogenic environmental pollutants, which occur in air, water, soils, sediments, in food and in the work area. Because many hundreds of closely related isomers are being formed and released in the environment from combustion processes of fossil fuels and other organic materials, their environmental and health control presents a difficult task.

Ideally, pure samples of each individual compound needing identification and quantitation should be available to the analyst for comparison and instrumental calibration. However, due to the enormous number of compounds which are encountered, this situation is unlikely to be attained in the foreseeable future. Instead, the widespread availability of high quality molecular spectra and related data represents a more realistic and practical alternative. For instance, UV and fluorescence spectra can facilitate determination by HPLC and low temperature fluorescence spectra can sometimes be used in Shpol'skii matrices to identify and determine certain isomers without prior separation. Mass spectra are of course extremely valuable for the combination of GC with MS, although isomer differentiation is not usually possible with this technique. For the unambiguous identification of isomers and metabolites, NMR spectra are very useful and IR spectra are traditionally valuable for "finger printing".

In order to obtain a data collection based on identical materials, all spectra were newly determined using samples of well defined purity. Table 1 gives an inventory of the materials studied in the order of presentation in this volume. Care was taken wherever possible to employ standard conditions for the measurement of the spectra. The range of solvents used was minimised and the concentrations and other operating conditions were kept approximately constant within a technique.

The present collection is the third volume published in the form of a "Spectral Atlas of PAC" and contains the spectra of 59 new compounds, i.e.

- 16 nitroderivatives of PAH
- 6 oxygenated heterocyclic PAC
- 15 sulfur-heterocyclic PAC
- 14 methylated or dimethylated PAH
- 8 metabolites (hydroxyderivatives)

In line with the first two volumes, the Atlas presents the following spectra, determined largely under standardised experimental conditions:

- UV-spectra
- Fluorescence and Phosphorescence Shpol'skii spectra at 15K

- Mass spectra (magnetic and quadrupole spectra)
- NMR spectra (proton- and carbon-13 spectra)
  IR-spectra taken in solution and in KBr pellets (including some Fourier transformation IR-spectra)

Following the example of the previous volumes, we have chosen to group all the spectra for each compound on consecutive pages, rather than keeping all spectra of the same type together as is common in data collections. We hope, hereby, to make the task of the user that much easier when seeking the available data on a particular compound.

Thus, the present volume extends the number of compounds covered by the Spectral Atlas of PAC to about 150, adding more than 500 spectra to the existing spectral collection. The range of compounds with additional data and information is extended to about 320 individual PAC.

With a view of facilitating the assessment of environmental and health hazards caused by this type of pollutants, this volume contains also an overview on the occurrence and biological activity of the various isomers treated. In addition, a special section reviewing the individual literature on the effects of approximately 150 PAC substances in the water environment is included, also. Further, this book contains information on essential physicochemical properties, for instance the octanol/water partition coefficient, HPLC retention indices, standard entropies and enthalpies and related properties.

W. Karcher
JRC Ispra
June 1991

2. Information for Users

A. Physicochemical Properties

A summary review of the 59 compounds considered in this volume is presented in table 1, which includes information on the chemical formula, mass number, melting point, purity, CAS-registry and BCR-reference material numbers.

Table 2 reports various physicochemical parameters determined for 56 Polycyclic Aromatic Compounds by high performance liquid chromatography (reversed phase) such as retention indices (I) and their standard deviation (I_n), retention times in minutes (t_{cm}) and their standard deviation (t_c); octanol/water partition coefficient (K_{ow}), water solubility (S), capacity factor (K'_n) and its standard deviation (k').

Liquid Chromatography on Reversed-Phase

Retention Indices

The retention characteristics of the PAC were determined on a polymeric VYDAK 201 TP (4.6 mm x 25 cm) column (The Separations Group, Hesperia, California). The retention data are presented as the logarithms of the retention indices. These retention indices were calculated as described by WISE and coworkers (1981, 1983). In this retention index system, the elution volume of the solute was measured simultaneously with the elution of standards (benzene, naphthalene, phenanthrene, benz(a)anthracene and benzo(b)chrysene), representing one to five condensed ring PAC. Acetone was used as non retained compound for the determination of the void volume. In the case of PAC eluted before benzene, the retention indices were extrapolated from the curve obtained between benzene and naphthalene.

The standards were assigned the following values (log I): benzene (1), naphthalene (2), phenanthrene (3), benz(a)anthracene (4) and benzo(b)chrysene (5). The retention index I was calculated using the following equation:

$$\log I_x = \log I_n + \frac{\log R_x - \log R_n}{\log R_{n+1} - \log R_n}$$

where X represents the solute, n and (n + 1) represent the lower and higher standards between which the compound elutes, and the R values the corresponding corrected retention volume (retention volume minus the void volume of the unretained acetone).

The mobile phase composition was mainly 85% acetonitrile in water. The mean reported log I_x is an average of three measurements.

Retention Times

The retention times have been reported as corrected retention times (minus the retention of the unretained acetone).

Capacity Factor K'

The capacity factor K' for one solute is defined as the ratio of the solute amount in the stationnary phase to the solute amount in the mobile phase. It can be determined experimentally by the following equation:

$$K' = \frac{C_s \times V_s}{C_m \times V_m} = K \cdot \frac{V_s}{V_m} = \frac{V_r - V_m}{V_m} = \frac{t_r - t_o}{t_o}$$

where V_s is the stationnary phase volume, V_m the mobile phase volume in the column, V_r the retention volume of the solute, C_s the concentration of the solute in the stationnary phase, C_m the concentration of the solute in the mobile phase, K the distribution coefficient between the phases ($K = C_s/C_m$), t_r the retention time of the solute, to the retention time of the acetone (unretained compound).

The reported values are an average of three measurements.

Octanol/Water Partition Coefficient log K_{ow}

Various publications have shown the relationships between retention time of a solute on reversed phase chromatography and the log K_{ow} (Swann et al., 1983; Weber et al., 1986; Chin et al., 1986; Andren et al., 1987). Octanol/water partition coefficients are estimated using a relatively simple relationship between K_{ow} and the corrected retention time t of the solute:

$$\log K_{ow} = A \log t + B$$

As for the retention index system, the coefficients A and B were calibrated by reference to the following standards (log K_{ow}): benzene (2.13), naphthalene (3.35), phenanthrene (4.57), benz(a)anthracene (5.87) and benzo(b)chrysene (7.11) (data from Karcher, 1988).

$$\log K_{ow} = \log (K_{ow_n}/K_{ow_{n+1}}) : (\log (t_n/t_{n+1}) \times \log_{tc} + (\log K_{ow_{n+1}}) (\log t_n) \cdot$$

$$\cdot (\log K_{ow_n}) (\log t_{n+1}) : \log (t_n/t_{n+1})$$

Table 1: Inventory of compounds

Nitro PAH

Compound	Chem Formula	Mass number	m.p. (°C)	Purity (%)	CAS Nr.	BCR - RM-Nr.
1-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	56.5	99.6	86-57-7	306
2-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	76	99.7	581-89-5	307
2-Methyl-1-nitronaphthalene	$C_{11}H_9NO_2$	187.20	81-82	99.3	881-03-8	
3-Nitrodiphenyl	$C_{12}H_9NO_2$	199.21	60	99.3	2113-58-8	
4-Nitrodiphenyl	$C_{12}H_9NO_2$	199.21	114	99.8	92-93-3	
5-Nitroacenaphthene	$C_{12}H_9NO_2$	199.21	101-2	83.6	602-87-9	
2-Nitrofluorene	$C_{13}H_9NO_2$	211.21	158	99.9	607-57-8	
9-Nitroanthracene	$C_{14}H_9NO_2$	223.23	146	99.7	602-60-8	308
2-Nitro-7-methoxy-naphtho(2,1-b)furan	$C_{13}H_9NO_4$	243.22	188	99.9	75965-74-1	312
3-Nitrofluoranthene	$C_{16}H_9NO_2$	247.26	166	99.8	892-21-7	310
1-Nitropyrene	$C_{16}H_9NO_2$	247.26	153	99.7	5522-43-0	305
9,10-Dinitroanthracene	$C_{14}H_8N_2O_4$	268.22	303-4	99.3	33685-60-8	
6-Nitrochrysene	$C_{18}H_{11}NO_2$	273.29	208	99.0	7496-02-8	309
7-Nitrobenz(a)anthracene	$C_{18}H_{11}NO_2$	273.29	161-2	99.9	20268-51-3	
6-Nitrobenzo(a)pyrene	$C_{20}H_{11}NO_2$	297.32	260	99.8	63041-90-7	311
3-Nitroperylene	$C_{20}H_{11}NO_2$	297.32	209	99.0	20589-63-3	

Oxygenated PAH

Compound	Chem Formula	Mass number	m.p. (°C)	Purity (%)	CAS Nr.	BCR - RM-Nr.
Dibenzo(b,d)furan	$C_{12}H_8O$	168.18	82.5	99.4	132-64-9	337
4-H-Cyclopenta(def)-phenanthren-4-one	$C_{15}H_8O$	204.21	171	99.7	5737-13-3	338
Benzo(b)naphtho(1,2-d)furan	$C_{16}H_{10}O$	218.24	44	99.9	205-39-0	340
Benzo(b)naphtho(2,1-d)furan	$C_{16}H_{10}O$	218.24	101-2	99.8	239-30-5	341
Benzo(a)fluorenone	$C_{17}H_{10}O$	230.25	133	99.8	76723-60-9	342
Benzo(c,d)pyren-6-one	$C_{19}H_{10}O$	254.27	243	99.4	3074-00-8	339

Sulfur-Heterocyclics

Compound	Chem Formula	Mass number	m.p. (°C)	Purity (%)	CAS Nr.	BCR - RM-Nr.
Dibenzothiophene	$C_{12}H_8S$	184.26	97	99.9	132-65-0	
1-Methyldibenzothiophene	$C_{13}H_{10}S$	198.27	67-9	90	31317-07-4	
2-Methyldibenzothiophene	$C_{13}H_{10}S$	198.27	84-5	94.4	20928-02-3	
3-Methyldibenzothiophene	$C_{13}H_{10}S$	198.27	77-9	90	16587-52-3	
4-Methyldibenzothiophene	$C_{13}H_{10}S$	198.27	66-7	98.0	7372-88-5	
Dibenzothiophenesulfoxide	$C_{12}H_8SO$	200.20	189	99.9	1013-23-6	
Dibenzothiophenesulfone	$C_{12}H_8SO_2$	216.24	234.6	99.9	1016-05-3	
Phenanthro(1,2-b)thiophene	$C_{16}H_{10}S$	234.30	169-70	95.2	58426-99-6	
Phenanthro(2,1-b)thiophene	$C_{16}H_{10}S$	234.30	237-8	98.5	219-25-0	
Phenanthro(3,4-b)thiophene	$C_{16}H_{10}S$	234.30	83	98.0	195-52-8	
Phenanthro(4,3-b)thiophene	$C_{16}H_{10}S$	234.30	94-5	99.8	195-68-6	
Phenanthro(9,10-b)thiophene	$C_{16}H_{10}S$	234.30	151-2	99.7	236-01-1	
7-Methylbenzo(b)-naphtho(2,3-d)thiophene	$C_{17}H_{12}S$	248.33	173-4	99.2	24964-09-8	
Benzo(b)naphtho-(1,2-d)thiophenesulfone	$C_{16}H_{10}SO_2$	266.30	235	99.9	20841-53-6	
Benzo(b)naphtho-(2,3-d)thiophenesulfone	$C_{16}H_{10}SO_2$	266.30	272	99.9	20841-57-0	

Methylated PAH

Compound	Chem Formula	Mass number	m.p. (°C)	Purity (%)	CAS Nr.	BCR - RM-Nr.
1-Methylfluorene	$C_{14}H_{12}$	180.24	85	99.4	1730-37-6	
4,5 Methylenephenanthrene	$C_{15}H_{10}$	190.23	114-5	99.0	203-64-5	
1-Methylphenanthrene	$C_{15}H_{12}$	192.25	123	99.7	832-69-9	
2-Methylphenanthrene	$C_{15}H_{12}$	192.25	58-9	98.7	2531-84-2	
3-Methylphenanthrene	$C_{15}H_{12}$	192.25	65	98.8	832-71-3	
4-Methylphenanthrene	$C_{15}H_{12}$	192.25	52-3	98.2	832-64-4	
9-Methylphenanthrene	$C_{15}H_{12}$	192.25	91-2	97.0	883-20-5	
9,10-Dimethylanthracene	$C_{16}H_{14}$	206.27	183-4	99.2	781-43-1	
9,10-Dimethylphenanthrene	$C_{16}H_{14}$	206.27	142-3	96.9	604-83-1	
1-Methylfluoranthene	$C_{17}H_{12}$	216.27	72-3	94.4	25889-60-5	
3-Methylfluoranthene	$C_{17}H_{12}$	216.27	66-8	99.9	1706-01-0	
7-Methylfluoranthene	$C_{17}H_{12}$	216.27	136-7	99.9	23339-05-1	
8-Methylfluoranthene	$C_{17}H_{12}$	216.27	93-4	99.0	20485-57-8	
4-Methylpyrene	$C_{17}H_{12}$	216.27	146	99.5	3353-12-6	

Metabolites

Compound	Chem Formula	Mass number	m.p. (°C)	Purity (%)	CAS Nr.	BCR - RM-Nr.
1-Hydroxyphenanthrene	$C_{14}H_{10}O$	194.22	154-5	99.2	2433-56-9	
2-Hydroxyphenanthrene	$C_{14}H_{10}O$	194.22	170-1	99.0	605-55-0	
3-Hydroxyphenanthrene	$C_{14}H_{10}O$	194.22	121	99.0	605-87-8	
4-Hydroxyphenanthrene	$C_{14}H_{10}O$	194.22	113-4	99.6	7651-86-7	
9-Hydroxyphenanthrene	$C_{14}H_{10}O$	194.22	149-50	99.2	484-17-3	
trans-9,10-Dihydroxy-9,10-dihydrophenanthrene	$C_{14}H_{12}O_2$	212.24	190-1	99.7	25061-77-2	
1-Hydroxypyrene	$C_{16}H_{10}O$	218.24	178-9	99.3	5315-79-7	
3-Hydroxybenzo(a)pyrene	$C_{20}H_{12}O$	268.30	214-6	99.8	13345-21-6	343

where n and n + 1 represent the lower and higher standards, t values are the corresponding corrected retention times, K_{ow} the octanol/water partition coefficient.

The reported mean value is an average of three measurements.

Water Solubility

Various models have been proposed for predicting water solubilities from octanol/water partitioning data (Yalkowski et al., 1979; Yalkowski and Valvani, 1980; Amidon and Williams, 1982). Doucette (1985) has established a regression curve obtained from 55 aromatic hydrocarbons:

$$\log S = -1.24 \log K_{ow} + 1.19 \text{ with } r^2 = 0.96$$

The presented calculated values for the PAC have been calculated from the above equation. Since calculated values are unreliable for most of compounds whose log K_{ow} exceeds 6, log S have not been calculated in these cases (4 compounds).

B. Occurrence

As a comprehensive assessment of the health effects of these important pollutants must be based on both occurrence and biological effects, a survey on the major sources and environmental distributions of PAH as well as an indication of their mutagenic and carcinogenic activities is included for each of the compounds. This review of the literature is not intended as an exhaustive survey but should facilitate the overall assessment of occurrence and of potential health risks.

The data are presented in tabulated format for convenience and grouped under four main headings:

- mobile sources (car exhaust, engine oils, crude oils)
- stationary sources (coal, oil, wood and peat combustion, coke ovens, tars, etc.)
- environmental domains (air, water, soil)
- foodstuffs (smoked meat, fish, vegetables, etc.)

C. Biological Activity

The biological data are summarised in tables 6 and 7, subdivided into bacterial mutagenicity data (Ames test) and animal carcinogenicity data (animal studies).

The data presented for the Ames test are based on results obtained with metabolic activation (S-9 mixture) and when comparing results of different origin, it should be born in mind that the purities and experimental conditions used in these tests can vary considerably.

D. Aquatic Toxicity

Anthropogenic PAH may reach the aquatic environment in industrial and domestic sewage effluents, surface runoff from land, deposition of airborne particulates, and spillage of petroleum and petroleum products into water bodies. Therefore, considerable interest has arisen concerning the study of the adverse effects of PAH on aquatic organisms and ecosystems. The information reviewed in this part gives the available scientific literature on this subject. The display of this information has been made in order to be understood by all the people (scientists, technologists, students...) interested in the biological effects of PAH in the aquatic and related environments.

Chemicals are arranged alphabetically by their common names whenever possible, or by their most commonly used trade names.

The Chemical Abstract Service (CAS) number follows the chemical name. The next entry is a summary table of ecotoxicity information.

The organisms are firstly arranged according to phylogenetic order and secondly alphabetically by their Latin scientific name (Genus and species). Endpoints are summarized by means of simple key words such as: survival (e.g.; LC50, LT50), growth (i.e.; inhibition or stimulation), respiratory responses (e.g.; gill exchange, oxygen uptake), reproduction (e.g.; fertilization, hatching success). These main key words, generally selected by the authors of the original publications, allow to rapidly obtain information on acute or chronic toxicity studies, laboratory or field experimentations. The last entry allows to retrieve the bibliographical references listed at the end of the book.

E. Spectral Measurements

1. Materials

A part of the compounds included in this volume were prepared in the context of an EC research and development programme for reference materials and applied metrology* (29-32). The materials were obtained by multistage synthesis and purification. Their preparation and purity characterization are described elsewhere (676). The purity of these reference materials is more than 0.99 g/g. The substances which where not available as reference materials were either obtained by purification of commercial materials or custom synthesized. All solvents used were spectroscopic grade and were mostly used without further purification.

* Certified reference materials are available from the EC Community Bureau of Reference (200, rue de la Loi, 1049 Brussels).

2. Measurement of Spectra

2.1 Ultraviolet Spectroscopy (UV)

The spectra were recorded on a model Uvikon 930 (Kontron Instruments). All spectra were measured at room temperature using fresh solutions prepared in spectroscopic grade cyclohexane. Solutions were measured in 1 cm quartz stoppered cuvettes against a reference of pure cyclohexane and spectra were recorded at spectral slit width of 1-2 nm, chosen, so as to achieve adequate resolution without sacrificing the signal to noise ratio, over the region 200-600 nm. The relatively weak region at long wavelengths was in same cases replotted with the ordinate scale multiplied by a factor of 10 or 5 to improve the utility of the spectrum as a reference.

2.2 Emission Spectroscopy

2.2.1 Room Temperature Fluorescence

Equipment

A SPEX 212 (FLUOROLOG 2) spectrofluorometer was used for room temperature fluorescence measurements. This spectrofluorometer was equipped with a Xenon lamp 450 W. Double monochromators were provided both for excitation and emission (focal distance 0.22 m), stepping motor for wavelength scanning. The slits were manually adjustable ranging from 0.02 nm to 15 nm. The sample compartment was thermostated at 20°C, with a simple beam excitation and an observation beam at right angle. The emission detector (HAMAMATSU R 928) was thermoelectrically cooled. Data acquisition and processing was computer controlled (80286 PC computer) through a SPEX DM 3000 software. The plot of the spectra was done through a ColorPro Hewlett Packard plotter.

Measurement Procedure

All the samples were dissolved in cyclohexane in a concentration range close to 5.10^{-7} mol/l, allowing the recording of reliable spectra, free of undesirable effects (scree effect, self absorption...). For some weak fluorescence emission compounds, higher concentration was used. Spectral slit widths were chosen according to the fluorescence properties of each compound, so as to provide a compromise between a good signal to noise ratio and maintaining the intrinsic resolution of the room temperature fluorescence bandwidths. All the spectra were recorded with an increment of 0.1 nm and an integration time of 0.5 s. The precision for the wavelength measurement of maxima was +/- 0.5 nm (for shoulder: +/- 1 nm).

Correction of the Fluorescence Emission Spectra

Each measured fluorescence intensity is multiplied by an instrumental correction factor Q(λ) stored in the computer system memory.

A calibrated tungsten lamp is used to determine the correction factors for wavelengths from 300 nm to 800 nm. For wavelengths lower than 300 nm we have used a Xenon lamp emission which was calibrated by extrapolation of its emission in the 300-400 nm range. These correction factors were further adjusted in order to reproduce the reference quinine sulfate spectrum provided by the National Institute for Standards and Technology (NIST, Gaithersburgh, MD).

Correction of the Fluorescence Excitation Spectra

This correction is realized in real time by means of a quantum counter constituted of a cell containing Rhodamine B and a photomultiplier placed on a reference beam. The sample signal intensity is first divided by the reference signal intensity provided by the quantum counter, and then the result is multiplied by a correction factor Qex(λ) which accounts for the difference between the two light paths.

For each molecule it was checked that the absorbance was sufficiently small at each wavelength to insure that the fluorescence intensity is a linear function of the absorbance i.e. $A = e(\lambda).c.l$, where $e(\lambda)$ is the molar absorption coefficient, c the molar concentration and l the optical path. The corrected fluorescence excitation spectrum should match with the absorption spectrum of the solute molecule.

2.2.2 High Resolution Shpol'skii spectrometry (HRS)

Low temperature emission (fluorescence and phosphorescence) spectra were recorded with a spectrofluorometer built from commercial components (Garrigues et al. 1981; 1983). Excitation was provided by the light of a Xenon lamp (XBO 450 W Osram) dispersed by a monochromator (model H 25, dispersion 3 nm/mm, Jobin-Yvon, Instruments S.A.) and focussed on the front surface of the polycrystalline solution to be analyzed.

Luminescence emission was observed at 90° through a one meter scanning spectrometer (model HR 1000, dispersion 0.8 nm/mm, Jobin-Yvon, Instruments S.A.) operating at a bandpass of 0.4 nm or 0.08 nm. Detection was provided by a photomultiplier (EMI 9789 QB) and spectra were stored on a hard disk of an IBM-XT microcomputer. Spectra were plotted on a 7074 A Hewlett Packard plotter.

Fused silica tubes containing the solutions of the aromatic compounds in n-alkanes (volume about 40 μl) were attached to the cold head of a closed cycle cryogenerator (CTI, Cryogenics 21 SC) operating at a temperature of 15 K. Preliminary fast freezing of the solutions at 77 K in liquid nitrogen gave satisfactory conditions for observing the Shpol'skii effect, i.e. well resolved emission spectra with bandwidths of the peaks of about 0.1 nm.

The concentration of the solutions of polycyclic aromatic compounds were adjusted at about 2 to $5x10^{-6}$ (i.e. below 1 mg/l). At this concentration level, the formation of aggregates is minimized and the reproducibility of fluorescence intensity is not altered (Garrigues et al., 1985a, 1985b).

For some weak emitting aromatic compounds (see below), a higher concentration was used in order to obtain a sufficient signal to noise ratio.

The choice of the n-alkane solvent is very important for the analysis of natural complex mixtures. The solvents were chosen so that the molecular dimensions of the aromatic molecules and the n-alkane chains were similar.

Several solvents were tested for all the studied aromatic compounds (n-hexane up to n-decane). However, n-alkanes with odd number of carbons were generally avoided (such as n-heptane, n-nonane) since their crystal lattice exhibits often more than one molecule per lattice and increases the number of possible substitutional sites i.e. the number of quasilines (Garrigues et al., 1983, 1985b).

The suitable Shpol'skii solvent for an aromatic compound was defined as producing well resolved spectra with a small number of quasilines. The presented spectra have been chosen according to this criterion after testing several solvents for a particular aromatic compound.

In the series where a phosphorescence or a fluorescence spectrum is not shown without any further information, this should be taken as evidence for the absence of such a spectrum under the experimental conditions used.

2.2.3 Particular Comments on the Analyzed Series

Nitro-PAH

These compounds do not exhibit any fluorescence emission at low temperature. The fluorescence emission of the 3-nitroperylene has not been recorded.

Oxygenated PAH

Furan derivatives exhibit both fluorescence and phosphorescence spectra. The three ketones of that series exhibit weak and broad band spectra adding no