ORGANIC ELECTRONIC
SPECTRAL DATA

Volume I   1946-1952

MORTIMER J. KAMLET, Editor

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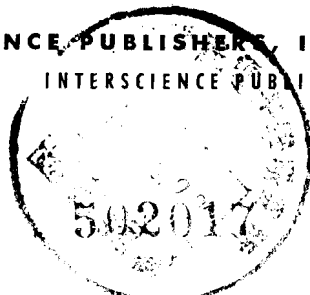
DEDICATORY PREFACE

E. A. Braude, 1922-1956

"The experimental technique of ultraviolet absorption spectroscopy has been developed to a high degree of perfection and standardization, a large volume of accurate data is now available, and the degree of specificity in the relation between structure and ultraviolet light absorption is of a suitable order for empirical interpretation."

These are the words of the late E. A. Braude in his lucid summary on ultraviolet light absorption and the structure of organic compounds (Annual Reports, Chem. Soc. London, 42, 105, 1945). It is thus fitting that the present catalog of spectral information be dedicated to him who was not only intensely interested in this field of correlation, but who also did much through his work to inspire others to appreciate the vanishing schism between preparative organic chemistry and physical measurements.

One of the many noteworthy contributions of Braude is the concept of the electron gas density as the "target area" for ultraviolet quanta (cf. Determination of Organic Structure by Physical Methods, E. A. Braude and F. C. Nachod, eds., Academic Press, New York, 1955, p. 135), the prediction of molar extinction on the basis of transition probability. This concept was cogently extended in his survey of stereochemical problems in general (Progress in Stereochemistry I, W. Klyne, ed., Academic Press, 1954, p. 126) and consideration of interplanar angles of substituted diphenyl in particular (cf. Experientia, 11, 457, 1955).

Ernest Braude was born in Germany and educated in England. His active scientific life was spent in the Imperial College of Science and Technology, London. His range of interests in organic chemistry was wide but his first and deepest scientific love was for the correlation of physical properties with chemical structure. In particular he became a recognized expert

in the field of ultraviolet spectroscopy. His researches in this and allied fields were intrinsi-
cally of the highest value. Perhaps even more important was the stimulus which he gave to
others by his writing and inspiring teaching.

He died in 1956 at the age of thirty-four. We dedicate this work to one who in a brief
span made a great contribution to the development of the subject.

R. P. Linstead
F. C. Nachod

INTRODUCTION TO THE SERIES

With the advent of photoelectric spectrophotometry, the volume of published ultraviolet spectral data increased sharply, quickly making the existing reference books obsolete and presenting Chemical Abstracts with a nearly impossible task. The need for collections of data was recognized by many workers and led to the publishing of catalogs of data in various fields (A.P.I., Friedel and Orchin, etc.) and a catalog of references (Hershenson). As yet, however, no comprehensive catalog of ultraviolet data has appeared.

In the spring of 1956 the editors of the present Volumes I and II envisaged, as a cooperative effort of a small group of chemists, a book reporting data for 1946-1955, found by a page by page search of journals. The enormity of the task undertaken was first realized when the number of journals covered passed 70 and the number of contributors (who reported 45,000 sets of data from 10,000 references and expended 5,500 hours) passed 50.

With the abundance of published data exceeding by far our initial expectations, it was deemed advisable to divide the compilation into two volumes, with one of us (MJK) accepting responsibility for Volume I (1946-1952) and the other (HEU) acting in the same capacity for Volume II (1953-1955).

In order to carry out this large effort efficiently and ensure its continuance, the group was incorporated as Organic Electronic Spectral Data, Inc., in May 1957. Officers and editors for Volumes I and II were elected and arrangements for supplements were put into effect.

Volume III, covering 1956-1957, is presently in preparation and will be edited by L. A. Kaplan and O. H. Wheeler. Abstracting for Volume IV covering 1958-1959 is almost complete. This volume will be edited by J. P. Phillips and F. C. Nachod. Volume V, which will cover 1960-1961, will be under the editorship of J. D. Cawley and R. E. Lyle.

H. E. Ungnade
M. J. Kamlet

PREFACE

The ultraviolet and visible spectra contained in this compendium were abstracted from the 1946-1952 volumes of over 60 chemical and allied journals. For inclusion it was necessary that data meet the following minimum requirements: (a) The investigated compound must be definable by a molecular formula and should be of sufficient purity to satisfy the usual analytical requirements. (b) Compounds of unknown structure must be sufficiently well described to be identifiable without recourse to the original literature. As examples, "carboxylic acid from chromic acid oxidation of jervine" is considered identifiable; "compound, m.p. 113°, from hydrolyzed barley extract" is not. (c) Wavelengths of maximal absorption and molar absorptivities must both be stated or determinable from information in the original paper. Several hundred articles listing positions of maxima without corresponding molar extinction coefficients were not abstracted for this reason. It is not necessary that the spectrum be completely described, however. If both λ_{max} and ϵ are given for one of several bands in the spectrum, the fragmentary information is considered to meet the requirement and is included. (d) During the course of the abstracting effort, several changes in policy were made with respect to data for which the solvent or phase was not specified, the final decision being to include such data with the notation n.s.g. (no solvent given) in the solvent column.

A very large portion of the effort involved in processing the data (arranging data cards in molecular formula order, converting nomenclature to a uniform system, encoding references, standardizing solvent and data entries, etc.) was carried out under contract at the Department of Organic Chemistry of the Hebrew University, Jerusalem, Israel, under the supervision of Dr. Ernst D. Bergmann. The editor is pleased to acknowledge the valuable contributions of Dr. Bergmann and of the other members of the staff and the students who participated in this phase of the operation.

Volumes I and II of the project were aided financially by American Cyanamid Company, Applied Physics Corporation, Beckman Instruments, Inc., and the Fisher Scientific Company to whom the editors wish to express their thanks. The editors also wish to express their gratitude to the National Science Foundation, whose generous grant made possible the processing of the data.

The editor of Volume I would be remiss if he did not acknowledge with gratitude the contributions of Mr. J. Hoffsommer, Mrs. Ruth B. Wheeler, Paula Heller, Mildred Sweitzer, and Rosalind G. Kamlet. Finally, thanks are due to the members of the staff of the Organic Chemistry Division, U. S. Naval Ordnance Laboratory, especially Dr. Darrell V. Sickman, for their sympathetic suggestions, assistance, and advice.

The fact that this is only Volume I of a continuing series provides a convenient mechanism for expanding and correcting the data herein published. Any errors or omissions, if communicated to the present editor, will be included in a corrected form in a subsequent volume. Cooperation by the reader in this continuing effort will be appreciated.

Mortimer J. Kamlet

U. S. Naval Ordnance Laboratory
Whiteoak, Silver Spring
Maryland
May 1960

ORGANIZATION AND USE OF THE DATA

Molecular Formula. The arrangement of compounds is according to molecular formulas and corresponds in most respects with that in the Chemical Abstracts Formula Index. As in Chemical Abstracts, the arrangement of symbols in formulas is alphabetical except that C always comes first, followed immediately by H if hydrogen is also present. The arrangement of formulas is also alphabetical except that the number of atoms of any specific kind dictates the order of compounds; e.g., all formulas with C (one carbon only) come before those with C_2; C_2H_2 precedes C_2H_3; C_2H_3Cl precedes $C_2H_3Cl_2$.

Simple salts and addition complexes are not given separate entries but are indicated in modifying phrases under the formulas of the compounds from which they are derived. Representative examples are:

> $C_7H_7NO_2$ (not $C_7H_6NNaO_2$)
> Benzoic acid, p-amino-, sodium salt,
>
> $C_8H_{11}N$ (not $C_8H_{11}NO_3S$)
> Aniline, N,N-dimethyl-, complex with sulfur trioxide,
>
> $C_9H_{12}N_2O_4S$ (not $C_9H_{13}ClN_2O_4S$)
> 4,5-Thiazoledicarboxylic acid, 2-amino-, diethyl
> ester, hydrochloride

The Chemical Abstracts method of indexing quaternary salts depends on whether or not the anionic moiety is specified in the original reference. Where specified, Chemical Abstracts lists the compound under the molecular formula of the salt; where not specified it is indexed as the corresponding quaternary hydroxide. Thus 3-methyl-1-phenyl-pyridinium bromide is indexed under $C_{12}H_{12}BrN$, the perchlorate under $C_{12}H_{12}ClNO_4$, the iodide under $C_{12}H_{12}IN$, but the cation (anion not specified) under $C_{12}H_{13}NO$, the listing in the latter case being: 3-Methyl-1-phenylpyridinium hydroxide, salt.

The present volume differs from the Chemical Abstracts Formula Index in that the latter system has been used in the indexing of all quaternary salts, irrespectively of whether or not the anion is specified. In the present volume the above four entries would be found together:

> $C_{12}H_{13}NO$
> 1-Phenylpyridinium hydroxide, 3-methyl-, hydro-
> bromic acid salt,
> 1-Phenylpyridinium hydroxide, 3-methyl-, hydriodic
> acid salt,
> 1-Phenylpyridinium hydroxide, 3-methyl-, perchloric
> acid salt,
> 1-Phenylpyridinium hydroxide, 3-methyl-, salt

The reasons for this departure from Chemical Abstracts' practice derive from the fact that the simple anions of most quaternary salts generally contribute little to their ultraviolet spectra. As a consequence the listing of all salts under a single molecular formula heading facilitates comparison of data and simplifies the search for spectra of such compounds. The reader need check only the single formula rather than the several required with the Chemical Abstracts system.

Compound Name. The arrangement of compound names under any molecular formula heading is generally alphabetic according to the preferred names of the isomers. All entries were checked against Chemical Abstracts' Annual Formula Indexes for 1946-1954 in an attempt to have nomenclature conform with the Chemical Abstracts system. For about 10%

of the entries the names may not correspond exactly. These include (a) the quaternary salts mentioned above, (b) compounds not listed by the Abstracts during this period, (c) situations where the Abstracts' name was in error, and (d) a few examples where the compound could be described in a less cumbersome manner.

Any nomenclature system must be flexible in order to meet new contingencies as they arise. The individual annual formula indexes of Chemical Abstracts may, for example, list similar compounds as derivatives of 5-pyrazolone or of 2-pyrazolin-5-one; as p-quinone, thio-; p-quinone, mercapto-; p-benzoquinone, thio-; or p-benzoquinone, mercapto-. No attempt has been made to resolve these differences in the present volume and, as a general rule, the name used corresponds with that in the most recent of the 1946-1954 annual indexes in which the specific compound is listed.

In many instances, such as the positioning of substituents in the more complex polycyclic systems, it was impossible to determine which of the various possible numbering systems the author used without referring back to the original article. This was done for most such entries, but the magnitude of the effort made it impractical to attempt it in all cases (see discussion of errors). It is therefore suggested that the reader go back to the original paper if the nomenclature is at all suspect.

Solvent. The solvent or phase (e.g., vapor) in which the spectrum was determined appears in the second column, abbreviated by a system which is essentially unambiguous but which, due to limitations of space, may often fail to describe the medium completely. For more complete descriptions of the solvent system the reader is referred to the original paper.

The following rules generally apply in the present volume: (a) Where a pH value or the concentration of acid, base, buffer, or salt is given, the solvent is understood to be water except in the case of NaOMe or NaOEt, where the solvent is the corresponding alcohol. (b) Where the original article specified both the pH value and the concentration of acid, base, or buffer, only the pH value is listed. (c) If the proportion of only one component of a binary system is specified, e.g., 50% dioxan, the other component is understood to be water. (d) H_2SO_4 generally denotes any concentration of sulfuric acid above 94%. Below this concentration the normality or proportion is specified or the abbreviation dil.H_2SO_4 is used. (e) Since many authors failed to specify the grade of alcohol used, it was decided to denote all concentrations of ethanol above 95% simply by EtOH. (f) For spectra determined at temperatures other than ambient, the temperature is given in the solvent column. (g) Molecular formulas of saturated paraffinic hydrocarbons and radical abbreviations denote the normal isomer unless otherwise specified. Thus C_5H_{12}, C_6H_{14}, C_7H_{16}, BuOAc, i-BuOH, and t-AmOH signify n-pentane, n-hexane, n-heptane, n-butyl acetate, isobutanol, and tertiary amyl alcohol, respectively. Some other common solvent abbreviations are listed in a separate section below.

Data Section. The numerical data in the third column represent wavelength values in millimicrons for all maxima, shoulders, and inflections, and the logarithms of the corresponding molar absorptivities in parentheses. Shoulders and inflections are denoted by the letter s following the wavelength. Where the original paper gives a range for λ_{max} the midpoint has been substituted.

Most of the compiled data are of two types: (a) Where numerical values of λ_{max} and and log ϵ or data from which these could be calculated (specific extinction, $E_{1cm}^{1\%}$, optical density plus concentration, etc.) were reported in the original reference, molar absorptivities are given to 0.01 logarithmic unit. (b) Where no such numerical data were reported and it was necessary to estimate either or both values from spectral curves, the molar absorptivity is given to only 0.1 logarithmic unit and both λ_{max} and log ϵ are underlined.

The chemical literature (especially the French and Russian) abounds in postage stamp sized spectral curves so poorly drawn or reproduced that independent abstracters, estimating from the same spectrum, will report the same maximum differing by as much as thirty millimicrons in position and as much as 0.3 logarithmic units in extinction coefficient. For this reason data in the latter category should be considered as being intrinsically far less reliable.

A smaller proportion of the data fall into two additional categories: (c) Data which are not underlined but in which extinction coefficients are given to only 0.1 logarithmic unit imply that numerical values of λ_{max} and log ϵ were reported, but that these values were insufficiently precise to warrant a second significant figure after the decimal point. (d) Logarithmic molar absorptivities given to 0.01 unit coupled with underlined data imply that the abstracter considered the spectrum sufficiently well drawn and his estimates sufficiently reliable to warrant inclusion of the additional significant figure. The reliability of such data should be treated with the same caution as that of category (b).

In estimating from spectral curves with superimposed fine structure, no attempt has been made to read all maxima. Only the main maximum or the center of the fine structure system is entered in such cases and labelled with the letter f after the wavelength. Where both numerical values and spectral curves were reported in the same paper, the numerical data have precedence and are reported as in category (a) with the values not underlined.

The abbreviation anom. (anomalous) has been used to denote any anomalies reported in the original paper. These include changing spectra due to chemical or photochemical transformations, thermochromism, failure to follow the Beer-Lambert relationship, or situations where graphical and numerical data in the same paper do not agree.

Reference. The final column lists the code number of the journal, the page number of the paper, and the last two ciphers of the year in which published (followed by a capital letter for journals issued in more than one volume per year). For example, the entry 33-0453-49 indicates that the information was abstracted from an article beginning on p. 453 of the 1949 volume of Journal No. 33 (Helvetica Chimica Acta). The complete reference (V. Prelog, K. Weisner, H. G. Khorana and G. W. Kenner, Helv. Chim. Acta, 32, 453 (1949), may be obtained by referring to the section at the end of the book which lists all articles abstracted. The journals are arranged in the order of their code numbers; the articles in the order of volume, year, and page.

Discussion of Errors. The abstractors have attempted to report faithfully the data from the original literature reference, and the data processors and the editor have collated this data, making necessary changes in nomenclature, etc.

Errata consist of two types, those perpetrated in the original literature and those arising during the process of translating the literature data into the present form. To demonstrate the former type, the spectrum of p-nitrophenol is not atypical. The following nine sets of λ_{max} (log ϵ) have been reported for the longer wavelength band of this compound in ethanol: 312(4.02), 314(4.11), 320(4.00), 315(4.0), 312(4.03), 310(3.97), 312(3.86), 312(3.99) and 308(4.1). Whether this range of data is caused by experimental errors or techniques or results from physical processes then not clearly understood is a moot point.

It should be emphasized that data are included even if known with absolute certainty to be incorrect. Such information may often be quite valuable by demonstrating the operation of otherwise unknown chemical or photochemical transformations. From comparison of values for aromatic Schiff bases, for example, it becomes apparent that as a result of hydrolysis by 5% water in 95% alcohol, many of the reported spectra represent composites of aldehyde, amine, and unreacted anil. Similarly, wide divergencies in reported spectra of nitrones point up a photochemical transformation of such compounds to oxaziranes. It

is suggested that comparisons of data in this and subsequent volumes may provide a point of departure for many fruitful research programs.

To evaluate errors of the second type, i.e., those for which the editors must accept responsibility, it is necessary to consider the magnitude of the effort involved in preparing the compilation. For Volumes I and II (1946-1952 and 1953-1955), fifty-two abstracters devoted over 6,500 man-hours to compiling over 50,000 sets of data from almost 10,000 references. In arranging the data cards in molecular formula and alphabetical order, converting nomenclature to the Chemical Abstracts system, encoding references, and standardizing solvent and data entries, an additional 6000 man-hours were expended by the data processing group at the Hebrew University. Typing rough and final drafts required a further several thousand hours.

Since ultimate responsibility for uniformity and accuracy rests with the editor, it is necessary to explain what has been done in the editing process. Optimally each entry would have been checked against the original reference to establish correctness of nomenclature and numerical data. This has been done in many instances, but no completeness can be claimed.

The editing operations performed and the principal errors still to be guarded against are as follows. Compound Name. Checking all entries again against the annual Chemical Abstracts Formula Indexes for 1946-1954 served to confirm most molecular formulas and nomenclature. The problems regarding numbering systems used by original authors have been mentioned in the section on organization and use of the data. Solvent: A uniform system of solvent abbreviations has been supplied. The abbreviation n.s.g. (no solvent given) occasionally appears where the solvent was indeed specified in the original paper but was missed by the abstracter as a result of its being so well hidden in the discussion. Data Section: The majority of undetected errors are in the data column. Few problems arose where molar absorbancy index or $\log \epsilon$ was specified in the original paper, but many mistakes were encountered where it was necessary to convert other measures of absorbancy to $\log \epsilon$. It was often quite difficult, for example, to ascertain whether the original authors had intended specific extinction coefficient or $E_1^{1\%}$cm. with the consequence that some values of $\log \epsilon$ are off by 1.0 logarithmic unit. Other values may be off by the logarithm of the molecular weight or log (mol. wt./10) as a result of confusion between molar and specific extinction coefficients or between ϵ and $E_1^{1\%}$cm. Detailed and often difficult calculations were required where I/I_0, per cent transmission, or per cent absorption plus concentration were specified. The earlier Russian literature abounds in a number of uncommon measures of absorbancy and for this reason should be particularly suspect. Directions regarding treatment of values estimated from curves were at times misinterpreted by a number of abstractors. As a result, underlining may sometimes not conform with the rules outlined in the section on organization and use of the data. Reference Section: Since any of the above-mentioned errors can readily be detected by referring to the original article, the greatest care was taken in checking all entries against the various journals or against Chemical Abstracts for correctness of the references.

PRINCIPAL ABBREVIATIONS

s	shoulder or inflection
f	fine structure
n. s. g.	no solvent given in original reference
anom.	anomalous spectrum (reader is referred to original reference)
C_5H_5N	pyridine
C_6H_6	benzene
C_6H_{12}	cyclohexane
C_7H_8	toluene
$C_2H_2Cl_4$	tetrachloroethane, generally the sym. isomer
DMF	dimethylformamide
pet. ether	petroleum ether, ligroin or any hydrocarbon mixture of unspecified composition
Mecyclo-hexane	methylcyclohexane
Isooctane	generally the commercial mixed hydrocarbons, but may be 2, 2, 4-trimethylpentane

JOURNALS ABSTRACTED

*Spectra issued in 1945 also included
**Contained no usable spectral data in 1946-52
***Continuation of Journal No. 53
****Spectra from the 1946-1952 volumes of this journal
will be included in "Organic Electronic Spectral Data, Volume III."

JOURNALS ABSTRACTED

Journal	Code No.	Journal	Code No.
Acta Chem. Scand.	1	Helv. Chim. Acta.	33
Acta Physicochim. U.S.S.S.	2	Ind. Eng. Chem.	34
Anal. Chem.	3	Izvest. Acad. Nauk S.S.S.R.,	
Anal. Chim. Acta	4	Otdel. Khim. Nauk	70
Ann. Chem. Liebigs	5	J. Am. Chem. Soc.	35
Ann. chim. (Paris)	6	J. Am. Pharm. Assoc., Sci.	
Ann. chim. (Rome)	7	Ed.	36
A. P. I. Research Project		J. Appli. Chem. (London)	69
No. 44*	8	J. Biol. Chem.	37
Appl. Spectroscopy	9	J. Chem. Phys.	38
Arch. Biochem.	10	J. Chem. Soc.	39
Arkiv Kemi	11	J. Chem. Soc. Japan	40
Atti accad. naz. Lincei	66	J. chim. phys.	41
Australian J. Sci.		J. Indian Chem. Soc.	42
Research	13	J. Opt. Soc. Amer.	43
Biochem. J	14	J. Org. Chem.	44
Biochem. Z.	15	J. Pharm. and Pharmacol.***	45
Biochim. et Biophys. Acta	71	J. Phys. Chem.	46
Bol. inst. quim. univ. na.		J. Polymer Sci.	47
auton. Me.	16	J. prakt. Chem.**	48
Boll. sci. fac. chim.		Monatsh. Chem.****	49
ind. Bologna	17	Nature	50
Bull. Chem. Soc. Japan	18	Naturwiss.	51
Bull. intern. acad.		Proc. Indian Acad. Sci.**	68
polon. sci.**	19	Proc. Iowa Acad. Sci.	67
Bull. soc. chim. Belges	20	Proc. Roy. Soc. (London)	52
Bull. soc. chim. biol.	21	Quart. J. Pharm. and	
Bull. soc. chim. France	22	Pharmacol.	53
Can. J. Chem.	23	Rec. trav. chim.	54
Chem. Ber.	24	Ricerca sci.	55
Chem. and Ind. (London)	25	Roczniki Chem.**	56
Chimia (Switz.)**	27	Science	57
Collection Czech. Chem.		Spectrochim. Acta**	59
Commun.	73	Trans. Faraday Soc.	60
Compt. rend.	28	Z. Elektrochem.	61
Discussions Faraday Soc.	29	Z. physik. Chem.	62
Doklady Akad. Nauk		Z. physiol. Chem.	63
S.S.S.R.	30	Z. Naturforsch.	64
Experientia	31	Zhur. Obshchei Khim.	65
Gazz. chim. ital.	32		

*Spectra issued in 1945 also included
**Contained no usable spectral data in 1946-52
***Continuation of Journal No. 53
****Spectra from the 1946-1952 volumes of this journal
will be included in "Organic Electronic Spectral Data, Volume III."

Compound	Solvent	λ_{max}(log ϵ)	Ref.
$CBrF_3$			
Methane, bromotrifluoro-,	gas	208 (1.52)	35-0467-51
CBr_2F_2			
Methane, dibromodifluoro-,	gas	227 (2.86)	''
CCIN			
Cyanogen chloride,	gas	featureless	38-0128-51
CCl_2F_2			
Methane, dichlorodifluoro-,	vapor	no maxima above 200	35-5486-50
CCl_3F			
Methane trichlorofluoro-,	vapor	no maxima above 200	''
CCl_4			
Carbon tetrachloride,	vapor	no maxima above 200	''
$CHBrF_2$			
Methane bromodifluoro-,	gas	no maxima above 208	35-0467-51
CHClO			
Chloroformaldehyde,	vapor or liquid	235 (1.70)	39-0948-46
$CHCl_2F$			
Methane, dichlorofluoro-,	vapor	no maxima above 200	35-5486-50
$CHCl_3$			
Chloroform,	vapor	no maxima above 200	''
CHI_3			
Iodoform,	$CHCl_3$	274 (3.0), 307 (3.2), 347 (3.2)	3-1473-51
CHN_5O_2			
Azidooxomethanediazonium hydroxide, hydrochloric acid salt,	H_2O	256s (2.2)	61-0383-49
CH_2Cl_2			
Methane, dichloro-,	vapor	no maxima above 200	35-5486-50

Compound	Solvent	λ_{max} (log ϵ)	Ref.
CH_2N_2			
Methane, diazo-,	gas	$\underline{380\,(0.5)}$, $\underline{408\,(0.5)}$, $\underline{435\,(0.5)}$	38 -1394 -51
CH_2N_4O			
Carbamyl azide,	EtOH	$\underline{233s\,(2.8)}$, $\underline{263s\,(1.8)}$	61 -0383 -49
CH_2N_6O			
Azidoiminomethanediazonium hydroxide, hydrochloric acid salt,	H_2O	$\underline{270s\,(2.2)}$	- ''
2H -Tetrazole -5 -diazonium hydroxide, hydrochloric acid salt,	H_2O	$\underline{263\,(3.4)}$	''
$CH_2N_6O_2$			
1H -Tetrazole, 5 -nitramino-,	H_2O	277 (4.14)	35 -2329 -51
1H -Tetrazole, 5 -nitramino-, potassium salt,	H_2O	$\underline{208\,(3.9)}$, 277 (4.15)	''
CH_2O			
Formaldehyde,	vapor or liquid	295 (1.0)	39 -0948 -46
	H_2O, 54°C	288 (1.13)	33 -1860 -47
CH_2O_2			
Formic acid,	vapor or liquid	205 (1.65)	39 -0948 -46
CH_3Br			
Methane, bromo-,	gas	204 (2.26)	35 -0467 -51
CH_3NO			
Formamide,	vapor or liquid	205s (2.20)	39 -0948 -46
CH_3NO_2			
Methane, nitro-,	EtOH	$\underline{269\,(1.2)}$	22 -0158 -50
	Isooctane	$\underline{273\,(1.2)}$, 278 (1.2), $\underline{286s\,(1.2)}$, $\underline{293s\,(1.1)}$	8 -0104 -45
CH_3N_5			
Formamidine, 1 -azido-, sulfate,	H_2O	$\underline{263s\,(1.8)}$	61 -0383 -49
2H -Tetrazole, 5 -amino-,	H_2O	featureless above 244	''
CH_4			
Methane,	gas	featureless 137-145.5	38 -0190 -50

Compound	Solvent	λ_{max} (log ϵ)	Ref.
CH₄N₂O			
Urea,	.1N NaOH	no maxima 220-250	35-0801-47
CH₄N₂O₂			
Methylamine, N-nitro-,	.005N HCl	232.5 (3.86)	23-0828-49
	.25N KOH	228 (3.88)	"
Methylamine, N-nitro-, potassium salt,	.1N HCl	230 (3.85)	35-1221-49
	1N NaOH	228.5 (3.88)	"
CH₄N₂S			
Urea, thio-,	EtOH	235 (4.04)	39-3722-52
Urea, thio-, Os(OH)Cl₅ complex,	.6M H₂SO₄	480 (3.6)	3-0317-50
Urea, thio-, complex with 4,6-dimethyl-2-pyrimidinethione,	EtOH	218 (4.01), 235 (3.96), 276 (4.08), 332 (3.41)	39-3722-52
CH₄N₄O₂			
Guanidine, nitro-,	H₂O	215 (3.75), 265 (4.15)	23-0828-49
	1N HCl	220 (3.7), 265 (4.1)	"
	1N HCl	220 (3.6), 265 (4.1)	23-0746-51
	1N KOH	256 (3.9)	"
	1N NaOH	252 (3.9)	23-0828-49
	EtOH	265 (4.18)	3-1740-51
	EtOH	212 (3.7), 262 (4.2)	23-0746-51
CH₄N₄O₄			
Methanediamine, N,N'-dinitro-,	.2N HCl	225 (4.1)	23-0828-49
	.2N NaOH	232.5 (4.23)	"
	EtOH	226 (4.10)	"
Methanedihydroxylamine, N,N'-dinitroso-,	1N HCl	231 (4.10)	"
	1N NH₄OH	255 (4.25)	"
Methanedihydroxylamine, N,N'-dinitroso-, ammonium salt,	H₂O	255 (4.2)	"
Methanedihydroxylamine, N,N'-dinitroso-, disodium salt,	H₂O	255 (4.2)	"
CH₄O			
Methanol,	liquid	featureless 220-405	8-0024-45
CH₅N₃			
Guanidine,	pH 1.04	featureless 220-250	35-0801-47
	pH 6.24	featureless 220-250	"
CH₅N₃O			
Semicarbazide, hydrochloride,	H₂O	278s (-0.7), 357s (-1.1)	61-0383-49

Compound	Solvent	λ_{max} (log ϵ)	Ref.
CH_5N_3S			
Semicarbazide, thio-,	H_2O	$\underline{235}$ (4.0)	37-0173-46C
	50% MeOH	$\underline{236}$ $\underline{(4.06}$)	35-2163-46
	MeOH	$\underline{242}$ $\underline{(4.1}$)	3-0384-51
	EtOH	$\underline{240}$ $\underline{(4.1}$)	22-0504-50
$CH_5N_5O_2$			
Guanidine, 1-amino-3-nitro-,	H_2O	214 (3.72), 267 (4.15)	35-2329-51
CH_6N_4			
Guanidine, 1-amino-,	EtOH	310s (1.3)	22-0446-52
Guanidine, 1-amino-, hydrochloride,	EtOH	$\underline{281}$ (0.2)	''
Guanidine, 1-amino-, nitrate,	EtOH	$\underline{297}$ (1.3)	''
Guanidine, 1-amino-, sulfate,	H_2O	$\underline{278}$s $\underline{(0.2}$)	61-0383-49