

INFRARED BAND HANDBOOK

Edited by

Herman A. Szymanski

~~Chairman~~, Chemistry Department
Canisius College

 PLENUM PRESS
NEW YORK • 1963

INTRODUCTION

Recent rapid advances in the techniques and instrumentation of infrared spectroscopy have made the determination of absorption spectra an increasingly more important and accurate method of analysis. However, the very refinements that have served to enhance the attractiveness of the method have also created the need for a greatly expanded information program. The Infrared Band Handbook is designed to play a many-sided role in this program. Perhaps its primary use will be in the identification of unknown compounds, but it will also be of value as a guide in assigning group frequencies, as a key to most advantageous sample conditions, as a tool in comparing series of related compounds for similar vibrations, and finally as an index to the literature.

The particular arrangement of the data that has been evolved is based on a number of premises:

1. That band position is the primary parameter for identifying unknown compounds from their infrared spectra. The identification of a compound from group frequencies alone is often difficult since many bands are not group frequencies.
2. That modern instrumentation and techniques make possible very accurate reporting of band position, and that, if the sample conditions are stated, this accuracy is reproducible.
3. That much of the literature does not report complete spectra, but concerns itself with the influences of physical and chemical changes on band position. This information is frequently lost to the spectroscopist.

The Handbook therefore presents data arranged by wavenumber, in steps of 1 cm^{-1} , and does not limit itself to complete spectra.

Sources

While the most accurate data are found in the current journals, it seemed desirable to include the widest selection of compounds in this initial volume. For this it was necessary to use data from older sources as well as from the current literature. This is especially true for many common organic compounds whose spectra have not been determined recently, but which form a necessary background, for instance, for the assignment of group frequencies.

The primary source of data for these common compounds was the American Petroleum Institute Project 44 series. This series represents accurate spectra of highly purified compounds, and therefore even early spectra of this group can be considered satisfactory. The Project 44 series, which shall be referred to as the API file, began issuing spectra in 1943. The file has been updated, and much of the early work has been redetermined quite accurately. However, some compounds have not been redetermined, and a few of these older entries have been included in the Handbook for completeness. It has been our experience in comparing these early data with those of later work that they are quite similar, except that the accuracy of the earlier work, especially in the $3600\text{--}2500\text{ cm}^{-1}$ region, is much lower. But all incorrect spectra have been replaced with other

data by the API workers. The only other source of older data has been several textbooks.

The remaining Handbook data have been taken from the literature published since 1957, although secondary references to earlier work will be found in the reference list. While the API file of course gives only complete spectra, data from the current literature may cover either single bands or the complete spectrum of a compound. In either case, only tabular data were used and in the interest of accuracy no attempt was made to measure band position in printed spectra. It should be noted that the ASTM indexing method utilized only printed spectra, so that in this respect the Handbook forms a complement to the ASTM index.

Accuracy of Band Position

As stated above, data have been entered in the Handbook in 1 cm^{-1} steps. While this arrangement is warranted by the accuracy of much of the information now being reported in the literature, we do not mean to imply this accuracy for all the data in the Handbook. A reasonable estimate of the accuracy of each entry can be made on basis of the date of the reference, the nature of the monochromator used, and the region of the spectrum involved. The following considerations will serve as a guide.

If the reference is of recent origin and only a NaCl prism spectrophotometer was used in the $3600\text{-}600 \text{ cm}^{-1}$ region, the accuracy of band position from 3600 to 2500 cm^{-1} can be assumed to range from $\pm 5 \text{ cm}^{-1}$ to $\pm 10 \text{ cm}^{-1}$. From 2500 cm^{-1} to 600 cm^{-1} the accuracy can be assumed to range from $\pm 5 \text{ cm}^{-1}$ to $\pm 1 \text{ cm}^{-1}$, with the higher accuracy corresponding to the lower wavenumbers. If the reference is to API data prior to 1950, the accuracy should be assumed to be even lower. For example, in the $3600\text{-}2500 \text{ cm}^{-1}$ region it probably is $\pm 10 \text{ cm}^{-1}$ unless a grating was used, in which case it would be closer to $\pm 5 \text{ cm}^{-1}$.

In general, where CaF_2 , LiF , or grating monochromators are used, the accuracy in the $3600\text{-}2500 \text{ cm}^{-1}$ region can be assumed to range from $\pm 5 \text{ cm}^{-1}$ to $\pm 1 \text{ cm}^{-1}$, i.e., to fall within the same limits assumed for the $2500\text{-}600 \text{ cm}^{-1}$ region. Some literature sources list the accuracy of their data, and this information is entered in the Handbook whenever it appeared pertinent.

Measured with a NaCl monochromator, many hydrocarbons have a series of common bands, particularly in the $3500\text{-}2000 \text{ cm}^{-1}$ region, where the band position cannot be measured as accurately as in the $2000\text{-}600 \text{ cm}^{-1}$ region. Obviously, these bands are not particularly useful for identification, and to conserve space in the Handbook, only some typical examples of such bands have been entered. The reader may assume that all compounds of the following types entered in the Handbook have the following bands in common:

| Band | Intensity | Path Length or Concentration | Physical State or Solvent |
|--|-----------|------------------------------|---------------------------|
| CH_3 and CH_2 Vibrations | | | |
| $3370 \pm 10 \text{ cm}^{-1}$ | MWSh | 0.169 | liquid |
| $3215 \pm 10 \text{ cm}^{-1}$ | SSh | 0.169 | liquid |
| $3180 \pm 10 \text{ cm}^{-1}$ | SSh | 0.169 | liquid |
| $2970 \pm 10 \text{ cm}^{-1}$ | S | 0.0088 | liquid |
| $2920 \pm 10 \text{ cm}^{-1}$ | S | 0.0088 | liquid |
| $2880 \pm 10 \text{ cm}^{-1}$ | S | 0.0088 | liquid |

| Band | Intensity | Path Length or Concentration | Physical State or Solvent |
|----------------------------|-----------|------------------------------|---------------------------|
| 2850 ± 10 cm ⁻¹ | S | 0.0088 | liquid |
| 2660 ± 10 cm ⁻¹ | MSSh | 0.169 | liquid |
| 2415 ± 10 cm ⁻¹ | M | 0.728 | liquid |
| 2320 ± 10 cm ⁻¹ | M | 0.728 | liquid |
| 2295 ± 10 cm ⁻¹ | S | 0.728 | liquid |
| OH of Alcohols | | | |
| 3350 ± 10 cm ⁻¹ | S | 5% | CCl ₄ |

Intensity Data

It is important for the reader to understand how intensity data were entered into the Handbook. Of all the information in the Handbook, intensity is the one most difficult to give in a generally meaningful way.

It is not intended for intensities of one compound to be compared to those of another, but only for intensities of all bands of a single compound to be compared to each other. Of course, in some instances different compounds can be compared to each other, but the reader should do this only after he has assured himself that the sample conditions were sufficiently similar to make the comparison meaningful.

The intensity data were prepared in the following manner. Where the source listed relative intensity for each band of a compound and only a single sample condition was used, the relative intensity data and physical conditions under which the sample was determined are listed. In general, no cell path length or concentrations are given unless such data are pertinent to band position. Where several path lengths or concentrations were used to complete the spectrum but the author has converted intensities to a relative scale, the relative intensity scale is used and concentrations and/or path lengths are not stated. API data presented a special problem since in many instances the sample had been determined using several path lengths and/or concentrations but no relative intensity data were given. For these spectra the intensity reported is that corresponding to the single concentration and/or path length which, in a given region of the spectrum, brings the greatest number of bands to an intensity from 5% to 95%. To indicate which bands are comparable in this situation, either the concentration or the path length is entered after the physical state code as an identifying mark. Since in this case either the path length or concentration is listed, but not both, the reader must consult the original reference for complete sample data.

Buffalo, N.Y.

H.A. Szymanski

EXPLANATION

The information listed to the left of the STRUCTURAL FORMULA of each compound has the following significance:

1 The first line gives the WAVE NUMBER in cm^{-1} and a code designation indicating the INTENSITY of the band (see Intensity Code below). For gases the band center or branch is identified whenever possible.

2 The second entry gives either a code letter indicating the PHYSICAL STATE in which the spectrum was measured (see Physical State Code below) or the solvent used for the sample (followed by the concentration, in brackets, and cell thickness, where pertinent).

The diagram shows two examples of spectral data entries. The first entry is: **989 S (R branch)** (1), **A (10 mm Hg, 10 cm)** (2), followed by the structural formula of 1,3-dioxolane. The second entry is: **986 M** (1), **E** (2), **Grating** (3), **[H₂CNO₂]⁻Na⁺** (4), **[CH₂ wag]** (5), and **328** (5) in the bottom right corner. A **201** (5) is also present between the two entries.

3 The next line is reserved for SPECIAL INFORMATION, such as the dispersive element used, the material of the prism, etc. In the absence of an entry the reader may assume that an NaCl prism was used.

4 The bracketed entry on the last line indicates the STRUCTURAL GROUP to which the vibration was assigned in the original reference, which may belong to either the original or the isomerized form of the compound, and the mode of vibration, where pertinent.

5 The number in the lower right-hand corner is the REFERENCE NUMBER and pertains to the list of source material on pages 429-434.

Intensity Code

(Intensity is described relative to all other bands in a given spectrum, except where it is necessary to use different path lengths and/or concentrations to record all bands. In such cases the path length and/or concentration is stated on the second line.)

S = Strong, **M** = Medium, **W** = Weak, **V** = Very, **B** = Broad, **Sh** = Shoulder, **Sp** = Sharp

Physical State Code

(The temperature is given after the code letter if it is other than 25°C.)

A = Vapor or gaseous state (followed by the pressure and path length, where pertinent)
B = Sample run as a liquid (followed by the cell thickness, in millimeters, where pertinent)
C = Solid, powder
D = Solid, film
E = Nujol oil
F = Fluorocarbon oil

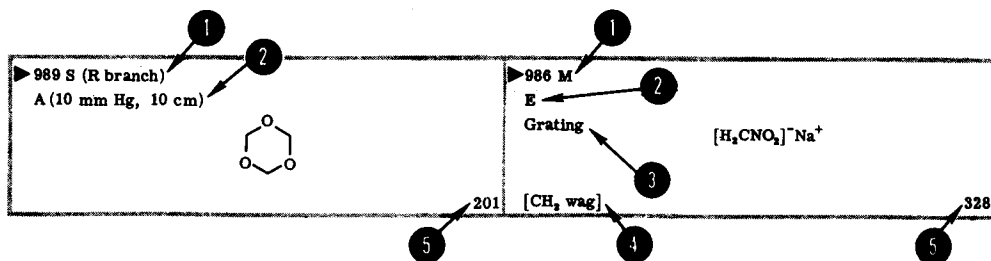
G = KBr disk
H = Solution — solvent not specified
I = Solid state — method not specified
K = Polyethylene bagging
M = Hexachlorobutadiene mull
N = Sample above room temperature and run as a liquid
O = Single crystal
P = KCl disk
Q = KI disk

EXPLICATION

Les renseignements situés à gauche de la FORMULE DE CONSTITUTION de chaque composé ont la signification suivante:

1 La première ligne donne l'INDICE DE L'ONDE en cm^{-1} et une désignation-code indiquant l'INTENSITE de la bande (voir Code-Intensité ci-dessous). Pour les gaz, le milieu de la bande ou l'embranchement est identifié quand c'est possible.

2 La seconde inscription donne soit une lettre-code indiquant l'ETAT PHYSIQUE dans lequel le spectre fut mesuré (voir Code-Etat Physique ci-dessous) ou le solvant utilisé comme échantillon, entre parenthèses, et la cellule épaisse, là où c'est à propos.



3 La ligne suivante est réservée pour des RENSEIGNEMENTS SPECIAUX, tels que l'élément du composé utilisé, la nature du prisme, etc. En l'absence d'une inscription, le lecteur peut assumer qu'on a employé un prisme NaCl.

4 L'inscription entre crochets de la dernière ligne indique le GROUPE DE CONSTITUTION auquel la vibration fut assignée dans la référence originale, laquelle peut appartenir ou à l'originale ou à la forme isomérisée du composé, et du genre du vibration, là où c'est à propos.

5 Le nombre qui se trouve à l'extrémité droite, en bas, est le NUMERO DE REFERENCE et se rattache à la liste de matériel source aux pages 429-434.

Code-Intensité

(L'intensité est décrite relative à toutes les autres bandes d'un spectre donné, sauf là où il faut s'en servir des différentes longueurs de traces et/ou des concentrations différentes pour enregistrer toutes les bandes. Dans de tels cas, la longueur de trace et/ou la concentration est donnée dans la seconde ligne.)

S = fort, M = moyen, W = faible, V = très, B = large, Sh = epaulement, Sp = aigu

Code-Etat Physique

(Si la température est autre que 25°C, elle est donnée après la lettre-code.)

A = Vapeur ou état gazeux (suivi de la pression et la longueur du trace, là où c'est à propos)

B = Echantillon éprouvé en tant que liquide (suivi de l'épaisseur de la cellule, en millimètres, là où c'est à propos)

C = Solide, en poudre

D = Solide, pellicule

E = Huile de Nujol

F = Huile de fluorocarbène

G = Disque KBr

H = Solution — solvant non spécifié

I = Etat solide — méthode non spécifié

K = Ensachement polyéthylène

M = Mélange hexachlorobutadiène

N = Echantillon au-dessus de la température normale d'intérieur et utilisé en tant que liquide

O = Cristal simple

P = Disque KCl

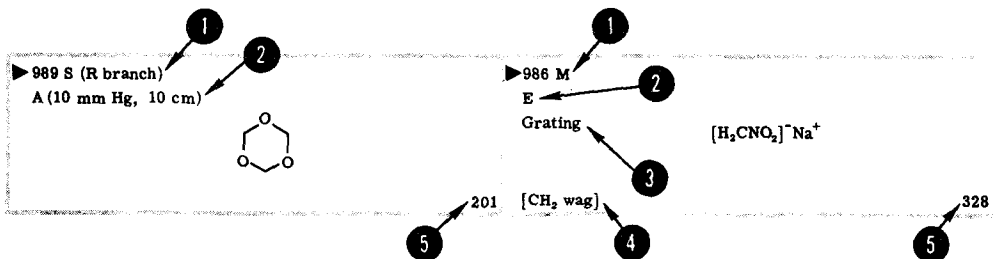
Q = Disque KI

ПОЯСНЕНИЯ

Слева СТРУКТУРНОЙ ФОРМУЛЫ каждого соединения приводятся данные, имеющие следующее значение:

1 На первой строке указываются **НОМЕР ВОЛНЫ** в см^{-1} и код, обозначающий **ИНТЕНСИВНОСТЬ** полосы. (См. ниже код интенсивности.) Для газов там, где это представляется возможным, обозначается центр или ветвь полосы.

2 На второй строке приводится буква кода, указывающая на **ФИЗИЧЕСКОЕ СОСТОЯНИЕ**, в котором измерялся спектр (см. ниже код физического состояния), или растворитель, применявшийся для пробы. Затем, в скобках, указывается концентрация, а там, где это существенно, толщина ячейки.



3 На следующей строке приводятся **ОСОБЫЕ ДАННЫЕ**, как-то: применявшийся элемент дисперсии, материал призмы и т. д. Если третья строка отсутствует, следует считать, что применялась призма NaCl.

4 На последней строке, в скобках, указывается **СТРУКТУРНАЯ ГРУППА**, к которой вибрация была отнесена в первоначальной ссылке. Эта группа может относиться к первоначальной или к изомеризованной форме соединения, а также там, где это существенно, к типу вибрации.

5 Номер, напечатанный справа внизу, является **НОМЕРОМ ССЫЛКИ**. Он относится к списку источников, упоминающихся на стр. 429-434.

Код интенсивности

(Интенсивность указывается в отношении всех прочих полос данного спектра, за исключением тех случаев, когда следует применять иные длины пробега и/или концентраций для записи всех полос. В таких случаях длина пробега и/или концентрации приводятся на второй строке.)

S = сильная, M = средняя, W = слабая, V = очень, B = широкая, Sh = плечо, Sp = острая

Код физического состояния

(Температура следует за буквой кода в том случае, если она не равняется 25°.)

A = Паро- или газообразное состояние (с указанием давления и длины пробега там, где это существенно)
 B = Проба в жидком состоянии (с указанием толщины ячейки в миллиметрах там, где это существенно)
 C = Твердое тело, порошок
 D = Твердое тело, пленка
 E = Масло Ньюжоль
 F = Фтороуглеродородное масло

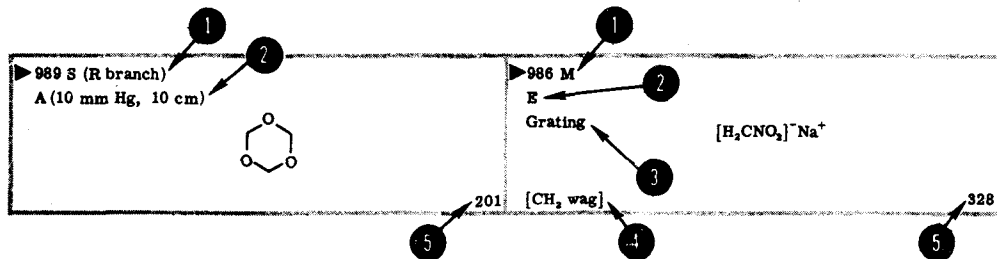
G = Диск КВг
 H = Раствор — без указания растворителя
 I = Твердое состояние — без указания метода
 K = Полиэтиленовая упаковка
 M = Шестихлоробутадиеновая смесь
 N = Температура пробы выше комнатной; проба в жидком состоянии
 O = Монокристалл
 P = Диск КСl
 Q = Диск КI

ERKLÄRUNG

Die links von der STRUKTURFORMEL einer jeden Verbindung stehenden Angaben haben die folgende Bedeutung:

1 Auf der ersten Zeile steht die WELLENZAHL in cm^{-1} sowie ein oder zwei Kennbuchstaben, die die INTENSITÄT des Bandes angeben (siehe Intensitäts-Kennbuchstaben unten). Nach Möglichkeit ist für Gase die Bandmitte oder jeweilige Bandseite mitgeteilt.

2 Die zweite Eintragung enthält entweder einen Kennbuchstaben, der den PHYSIKALISCHEN ZUSTAND bezeichnet, in dem das Spektrum ermittelt wurde (siehe Zustands-Kennbuchstaben unten), oder das für die Probe benutzte Lösungsmittel (sowie nachstehend die Konzentration in eckigen Klammern und die Zellendicke, falls zutreffend).



3 Die nächste Zeile ist für BESONDERE ANGABEN vorbehalten, wie z. B. das benutzte Dispersionselement, das Prismenmaterial usw. Sofern keine Angaben gemacht sind, kann der Leser annehmen, dass ein NaCl-Prisma benutzt wurde.

4 Die Eintragung in eckigen Klammern auf der letzten Zeile gibt die STRUKTURGRUPPE an, der die Schwingung im Originalbericht zugeeignet worden war—diese kann entweder der ursprünglichen oder der isomeren Form der Verbindung angehören —, sowie die Schwingungsart, falls zutreffend.

5 Die Zahl in der rechten unteren Ecke stellt die BEZUGSZAHL dar und bezieht sich auf die Quellenliste auf S. 429-434.

Intensitäts-Kennbuchstaben

(Die Einstufung der Intensität bezieht sich auf alle anderen Bänder eines gegebenen Spektrums, ausser in Fällen, wo verschiedene Bahnlängen und/oder Konzentrationen erforderlich waren, um alle Bänder zu erfassen. In diesen Fällen sind Bahnlänge und/oder Konzentration auf der zweiten Zeile angegeben.)

S = Stark, M = Mittel, W = Schwach, V = Sehr, B = Breit, Sh = Schulter, Sp = Scharf

Zustands-Kennbuchstaben

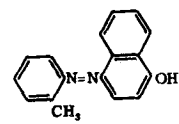
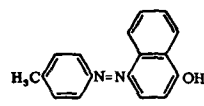
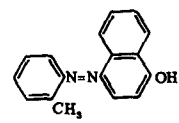
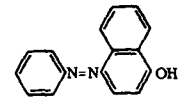
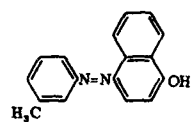
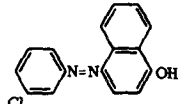
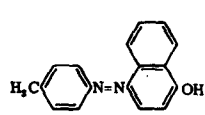
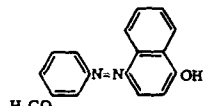
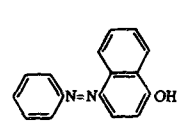
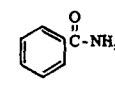
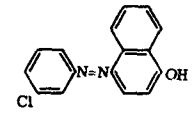
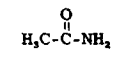
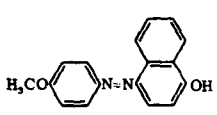
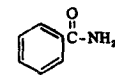
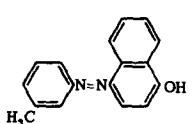
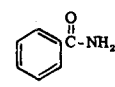
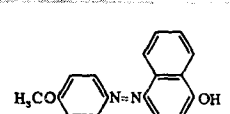
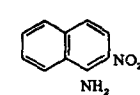
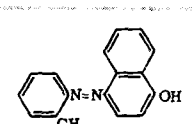
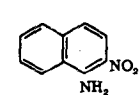
(Die Temperatur ist nach dem Kennbuchstaben angeführt, falls sie nicht 25°C betrug.)

A = Dampf- oder Gaszustand (dahinter Druck und Bahnlänge, falls zutreffend)
 B = Prüfung erfolgte im flüssigen Zustand (dahinter die Zellendicke, falls zutreffend)
 C = Festzustand, pulverförmig
 D = Festzustand, Filmform
 E = Nujol-Öl
 F = Fluorkohlenstoff-Öl
 G = KBr-Scheibe

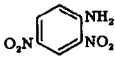



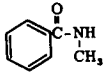

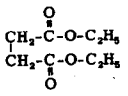
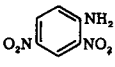




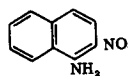

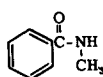

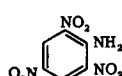

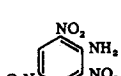
H = Lösung—Lösungsmittel nicht angegeben
 I = Festzustand—Methode nicht angegeben
 K = Polyäthylen-Beutel
 M = Hexachlorbutadien-Mull
 N = Prüfung oberhalb Zimmertemperatur im flüssigen Zustand
 O = Einkristall
 P = KCl-Scheibe
 Q = KI-Scheibe

CONTENTS

| | |
|---|-----|
| Introduction | vi |
| Explanation | |
| in English | ix |
| in French | x |
| in Russian | xi |
| in German | xii |
| Infrared Absorption Bands | 1 |
| References | 429 |
| Index | 435 |
| Appendix I. Correlation Tables for Methyl Deformation Frequencies . . . | 465 |
| Table I. Methyl—Carbon Frequencies | 466 |
| Table II. Methyl—Silicon Frequencies | 468 |
| Table III. Methyl—Nitrogen Frequencies | 469 |
| Table IV. Methyl—Phosphorus Frequencies | 470 |
| Table V. Methyl—Boron Frequencies | 470 |
| Table VI. Methyl—Oxygen Frequencies | 471 |
| Table VII. Methyl—Sulfur Frequencies | 472 |
| Table VIII. Methyl—Halogen Frequencies | 473 |
| Table IX. Methyl—Metal Frequencies | 474 |
| Summary | 475 |
| Conclusions | 476 |
| Bibliography | 477 |
| Appendix II. Correlation Tables for C—N Stretching Frequencies | 479 |
| Table I. Primary Aliphatic Amines | 480 |
| Table II. Secondary Aliphatic Amines | 480 |
| Table III. Nitro—Alkanes | 481 |
| Table IV. Compounds Containing CH ₃ —N Group | 481 |
| Table V. C—N $\begin{matrix} \diagup O \\ \diagdown \end{matrix}$ in Ring Compounds | 481 |
| Table VI. HN=C—N Group in Acetamidines | 482 |
| Table VII. Some Ethanamides (Amido Group) | 482 |
| Table VIII. C _{alk} —N Stretching Frequencies of Acetamidines | 482 |
| Table IX. General Ranges of C—N Vibration in Various Compounds | 482 |
| Table X. Nitro Group Attached to Monophenyl Ring | 483 |
| Table XI. Nitro Group Attached to Diphenyl Ring | 483 |
| Table XII. Secondary Aromatic Amines | 483 |
| Table XIII. Amide II Band | 483 |
| Bibliography | 484 |

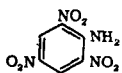
| | |
|---|--|
| <p>▶ 3610 S C₆H₁₃, C₂Cl₄</p>  <p>[OH] 35</p> | <p>▶ 3570 MS CHCl₃</p>  <p>[OH] 35</p> |
| <p>▶ 3600 S CCl₄</p>  <p>[OH] 35</p> | <p>▶ 3570 MS CHCl₃</p>  <p>[OH] 35</p> |
| <p>▶ 3580 S CH₂Cl₂</p>  <p>[OH] 35</p> | <p>▶ 3570 VW CHCl₃</p>  <p>[OH] 35</p> |
| <p>▶ 3580 S CH₂Cl₂</p>  <p>[OH] 35</p> | <p>▶ 3560 M CH₂Cl₂, CHCl₃</p>  <p>[OH] 35</p> |
| <p>▶ 3580 S CH₂Cl₂</p>  <p>[OH] 35</p> | <p>▶ 3540 MW CCl₄</p>  <p>29</p> |
| <p>▶ 3580 M CH₂Cl₂</p>  <p>[OH] 35</p> | <p>▶ 3538 CHCl₃</p>  <p>474</p> |
| <p>▶ 3575 S CH₂Cl₂</p>  <p>[OH] 35</p> | <p>▶ 3525 MW CHCl₃</p>  <p>29</p> |
| <p>▶ 3575 MS CHCl₃</p>  <p>[OH] 35</p> | <p>▶ 3520 MW CCl₄</p>  <p>29</p> |
| <p>▶ 3570 S CHCl₃</p>  <p>[OH] 35</p> | <p>▶ 3520 MW CCl₄, CaF₂</p>  <p>[NH₂] 19</p> |
| <p>▶ 3570 MS CH₂Cl₂, CHCl₃</p>  <p>[OH] 35</p> | <p>▶ 3519 CHCl₃, CaF₂</p>  <p>[NH₂] 19</p> |

| | | | |
|---|-----|---|-----|
| ▶3517 CCl ₄ CaF ₂ | | ▶3501 MW C ₆ H ₅ CaF ₂ | |
| [NH ₂] | 19 | [NH ₂] | 19 |
| ▶3516 M CCl ₄ | | ▶3501 MW C ₆ H ₅ CaF ₂ | |
| [OH] | 475 | [NH ₂] | 19 |
| ▶3516 Sh CHCl ₃ CaF ₂ | | ▶3500 C ₆ H ₅ CaF ₂ | |
| [NH ₂] | 19 | [NH ₂] | 19 |
| ▶3511 M CCl ₄ , CHCl ₃ CaF ₂ | | ▶3500 | |
| [NH ₂] | 19 | | 465 |
| ▶3511 CHCl ₃ CaF ₂ | | ▶3497 MW C ₆ H ₅ NO ₂ CaF ₂ | |
| [NH ₂] | 19 | [NH ₂] | 19 |
| ▶3510 CHCl ₃ , CCl ₄ | | ▶3495 C ₇ H ₇ N CaF ₂ | |
| | 327 | | 19 |
| ▶3510 CHCl ₃ | | | |
| | 327 | | |
| ▶3507 M CCl ₄ | | ▶3490 C ₆ H ₅ NO ₂ CaF ₂ | |
| [OH] | 475 | [NH ₂] | 19 |
| ▶3504 | | ▶3488 W C ₇ H ₇ N CaF ₂ | |
| | 477 | [NH ₂] | 19 |
| ▶3504 MW (C ₂ H ₅) ₂ O CaF ₂ | | ▶3487 MW CH ₃ CN CaF ₂ | |
| [NH ₂] | 19 | [NH ₂] | 19 |
| ▶3504 Sh (C ₂ H ₅) ₂ O CaF ₂ | | ▶3487 Sh CHCl ₃ CaF ₂ | |
| [NH ₂] | 19 | [NH ₂] | 19 |

| | |
|---|--|
| <p>▶ 3484 M C₅H₅NO₂ CaF₂</p>  <p>[NH₂]</p> | <p>▶ 3475 S CCl₄ CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3481</p>  <p>479</p> | <p>▶ 3475 M C₆H₆ CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3480 W CCl₄ [0.3 g/ml]</p>  <p>2</p> | <p>▶ 3474 M C₅H₅N CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3480</p>  <p>[C=O overtone]</p> <p>478</p> | <p>▶ 3474 MW CH₃CN CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3480 CHCl₃, CCl₄ CaF₂</p>  <p>[NH₂]</p> <p>470</p> | <p>▶ 3473 M C₆H₅NO₂ CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3479 MW (C₂H₅)₂O CaF₂</p>  <p>[NH₂]</p> <p>49</p> | <p>▶ 3470</p> <p>CH₃NH₂</p> <p>480</p> |
| <p>▶ 3478 S CHCl₃ CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3464 MW CH₃CN CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3478 M CH₃CN CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3460 W CCl₄ [0.007 g/ml]</p>  <p>[NH]</p> <p>2</p> |
| <p>▶ 3477 M (C₂H₅)₂O CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3457 MS C₂Cl₄, CHCl₃ CaF₂</p>  <p>[NH₂]</p> |
| <p>▶ 3476 S C₂Cl₄ CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3457 M CH₃CN CaF₂</p>  <p>[NH₂]</p> |

3456

▶ 3456 S
C₆H₆
CaF₂



[NH₂]

19

▶ 3420 M
CHCl₃



327

▶ 3420
CCl₄



327

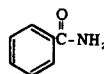
▶ 3455 MW
C₂H₅N
CaF₂



[NH₂]

19

▶ 3420 MW
CCl₄



29

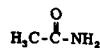
▶ 3454
CHCl₃
CaF₂



[NH₂]

470

▶ 3420
CHCl₃



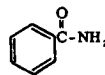
474

▶ 3450 M
E



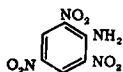
327

▶ 3410 M
CHCl₃



29

▶ 3450 Sh
C₄H₉N
CaF₂
CaF₂



[NH₂]

19

▶ 3401 MS
CCl₄ [5%]



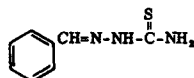
318

▶ 3450



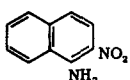
483, see also 36, 44, 482

▶ 3400 S



380

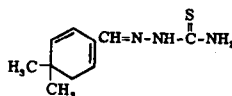
▶ 3443 M
(C₂H₅)₂O
CaF₂



[NH₂]

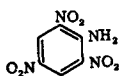
19

▶ 3400 S



380

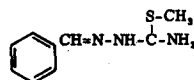
▶ 3437
P
CaF₂



[NH₂]

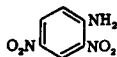
19

▶ 3400 S



380

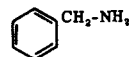
▶ 3435 M
C₂H₅N
CaF₂



[NH₂]

19

▶ 3400



383

▶ 3435 M
E

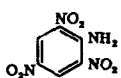


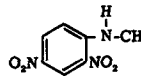
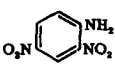
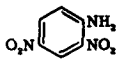


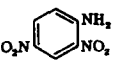
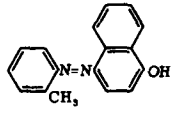

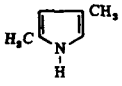
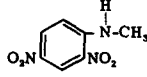
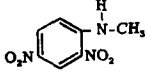
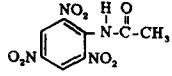
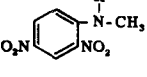
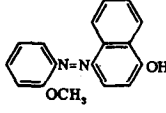


327

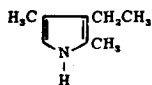
▶ 3400
CHCl₃



327

| | |
|---|--|
| <p>▶ 3395 MW C₆H₅N</p>  <p>19</p> | <p>▶ 3383 MW C₆H₅N CaF₂</p>  <p>[NH₂] 19</p> |
| <p>▶ 3394 CCl₄ CaF₂</p>  <p>[NH₂] 470</p> | <p>▶ 3382 M CH₃CN CaF₂</p>  <p>19</p> |
| <p>▶ 3393 CCl₄ CaF₂</p>  <p>[NH₂] 19</p> | <p>▶ 3381 C₆H₅ CaF₂</p>  <p>[NH₂] 19</p> |
| <p>▶ 3392 M (C₂H₅)₂O, CCl₄, CHCl₃ CaF₂</p>  <p>[NH₂] 19</p> | <p>▶ 3381 M C₆H₅NO₂ CaF₂</p>  <p>[NH₂] 19</p> |
| <p>▶ 3391 MS CCl₄ [5%]</p> <p>CH₃CH₂C(CH₃)₂OH</p> <p>194</p> | <p>▶ 3380 MWSh B (0.169)</p> <p>(CH₃)₂CHCH(CH₃)₂ CH₂ CH₃</p> <p>301, see also 472</p> |
| <p>▶ 3391 CHCl₃ CaF₂</p>  <p>[NH₂] 19</p> | <p>▶ 3380 MW CCl₄</p>  <p>[NH] 35</p> |
| <p>▶ 3388 M C₆H₅ CaF₂</p>  <p>[NH₂] 19</p> | <p>▶ 3380 MSh A</p> <p>H-C≡C-C(=O)-H</p> <p>18</p> |
| <p>▶ 3385 VVS B (0.055) CaF₂</p>  <p>344</p> | <p>▶ 3380 VS CHCl₃ CaF₂</p>  <p>[NH] 19</p> |
| <p>▶ 3384 S C₆H₅ CaF₂</p>  <p>[NH] 19</p> | <p>▶ 3380 M CCl₄, C₆H₅, CHCl₃ CaF₂</p>  <p>[NH] 19</p> |
| <p>▶ 3383 S CCl₄ CaF₂</p>  <p>[NH] 19</p> | <p>▶ 3380 M C₆H₁₂</p>  <p>[NH] 35</p> |

▶3379 VVS
B (0.055)
CaF₂



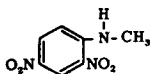
343

▶3367 S
CCl₄ [5%]



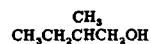
195

▶3378 M
C₆H₅NO₂
CaF₂



19

▶3367 MS
CCl₄ [25%]



321

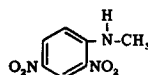
[NH]

▶3376
CHCl₃
CaF₂



470

▶3365 M
(CH₃)₂CO
CaF₂



[NH]

19

▶3373 MW
CH₃CN



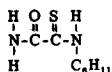
19

▶3364 M
CHCl₃
CaF₂

[NH₂]

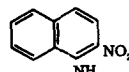
19

▶3372 MS
G



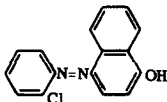
31

▶3363 MW
CHCl₃
CaF₂

[NH₂]

19

▶3370 M
C₆H₁₂, CCl₄, C₂Cl₄



35

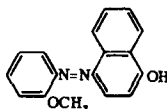
▶3362 M
C₆H₅, C₆H₅NO₂, (C₂H₅)₂O
CaF₂



[NH]

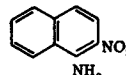
19

▶3370 M
C₂Cl₄, CCl₄



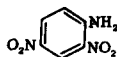
35

▶3362 M
CCl₄, C₆H₆
CaF₂

[NH₂]

19

▶3368 S
C₆H₅NO₂
CaF₂



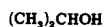
19

▶3361 M
C₂Cl₄
CaF₂

[NH₂]

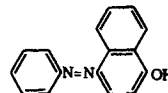
19

▶3367 VS
V



460

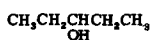
▶3360 W
CH₂Cl₂, CHCl₃



[NH]

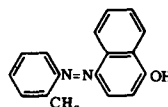
35

▶3367 VS
CCl₄ [5%]



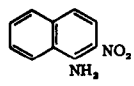
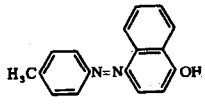
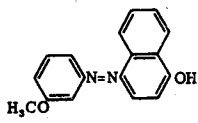
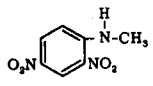
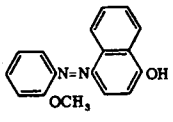
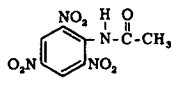
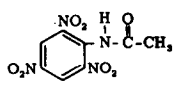

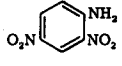

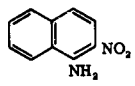
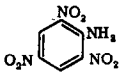
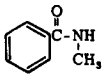

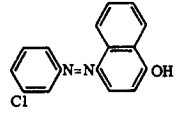

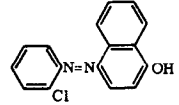
198

▶3360 W
CH₂Cl₂, CHCl₃

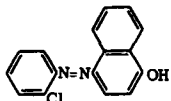


[NH]

35

| | |
|--|--|
| <p>▶ 3360 M C₉H₇NO₂ CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3350 M CH₂Cl₂, CHCl₃</p>  <p>[NH]</p> <p>35</p> |
| <p>▶ 3360</p> <p>CH₃NH₂</p> <p>480</p> | <p>▶ 3350 M CH₂Cl₂, CHCl₃</p>  <p>[NH]</p> <p>35</p> |
| <p>▶ 3360 MW C₈H₈N CaF₂</p>  <p>[NH]</p> <p>19</p> | <p>▶ 3350 MS CH₂Cl₂</p>  <p>[NH]</p> <p>35</p> |
| <p>▶ 3359 MW C₈H₈NO₂ CaF₂</p>  <p>[NH]</p> <p>19</p> | <p>▶ 3349 MW CH₃CN CaF₂</p>  <p>[NH]</p> <p>19</p> |
| <p>▶ 3358 M C₆H₇N CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3348 MS CH₃CN CaF₂</p>  <p>[NH₂]</p> <p>19</p> |
| <p>▶ 3358 M CCl₄ CaF₂</p>  <p>[NH₂]</p> <p>19</p> | <p>▶ 3348 M CH₃CN CaF₂</p>  <p>[NH₂]</p> <p>19</p> |
| <p>▶ 3356 VS CCl₄ [5%]</p> <p>CH₃CH₂CH₂OH</p> <p>314</p> | <p>▶ 3344 MS CHCl₃, C₂Cl₄, C₆H₆ CaF₂</p>  <p>[NH₂]</p> <p>19</p> |
| <p>▶ 3350 W CCl₄ [0.007 g/ml]</p>  <p>[NH]</p> <p>2</p> | <p>▶ 3343 MW (C₂H₅)₂O CaF₂</p>  <p>[NH₂]</p> <p>19</p> |
| <p>▶ 3350 M CH₂Cl₂</p>  <p>[NH]</p> <p>35</p> | <p>▶ 3342 Sh (C₂H₅)₂O CaF₂</p>  <p>[NH₂]</p> <p>19</p> |
| <p>▶ 3350 M CH₂Cl₂</p>  <p>[NH]</p> <p>35</p> | <p>▶ 3340 MSh B (0.169)</p> <p>(CH₃)₂CHCH₂CH₂CH(CH₃)₂</p> <p>137, see also 339</p> |

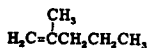
▶3340 M
E, G, CHCl₃



[NH]

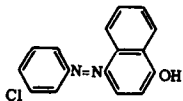
35

▶3340 VS
B (0.169)



206

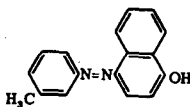
▶3340 M
CHCl₃



[NH]

35

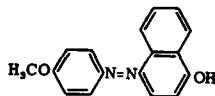
▶3340 W
CH₂Cl₂, CHCl₃



[NH]

35

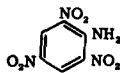
▶3340 W
CH₂Cl₂, CHCl₃



[NH]

35

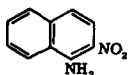
▶3339 M
CH₃CN
CaF₂



[NH₂]

19

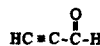
▶3336 M
(C₂H₅)₂O
CaF₂



[NH₂]

19

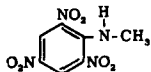
▶3335 VS
A



[=CH]

18

▶3334 M
CHCl₃, C₆H₆
CaF₂



[NH]

19

▶3334
E, CHCl₃



[NH₂]

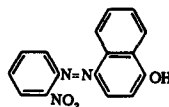
327

▶3334
CCl₄



327

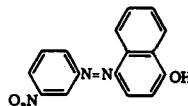
▶3330 MS
C₂Cl₄



[NH]

35

▶3330 M
CHCl₃



[NH]

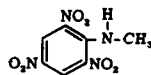
35

▶3330 M
E



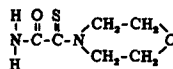
327

▶3329 M
P, CH₃CN, C₂H₅N
CaF₂



19

▶3325 S
G



[NH]

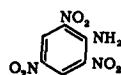
31

▶3325
A



485

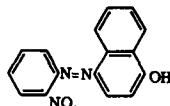
▶3321 M
P
CaF₂



[NH₂]

19

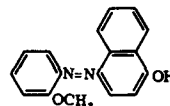
▶3320 MS
E, G, CH₂Cl₂



[NH]

35

▶3320 M
E, G



[NH]

35

▶3320
E, CHCl₃



327