INFRARED BAND HANDBOOK

SUPPLEMENTS 3 & 4

Edited by Herman A. Szymanski
Chairman, Chemistry Department
Canisius College

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INTRODUCTION

In the initial volume of this series infrared data for the 3600-600 cm^{-1} wavenumber range were taken from API Project 44 spectra, from textbooks, and from periodicals. This provided a wide variety of spectra, run over a period of several years. Supplements 1 and 2, using essentially the same sources, extended the tabulation into the 700-0 cm^{-1} range. The present volume, which covers the entire wavelength range, is the first one to present data from only the current periodical literature. Since research reports published in most journals are subject to a painstaking review process, it can generally be assumed that the work was performed on very accurate instruments and with high-purity compounds, and that the data reported are therefore accurate and reliable. It is an established fact that, given the same sample conditions, workers in different laboratories using modern high-resolution instruments are consistently capable of determining band positions to within 1 cm^{-1}.

This accuracy strengthens the very concept on which the Infrared Band Handbook is based—the reporting of data by band position. Still, I suggest that in comparing the spectrum of an unknown with the data in the Handbook, the reader check bands within 2-5 cm^{-1} of the position of the band in his spectrum. This range should be sufficient to allow for variations due to slight differences in experimental conditions.

It may be useful here to restate my reasons for preparing the Infrared Band Handbook series. The most important information obtained from an infrared spectrum is the position of the absorption bands. Frequently journal articles deal with only a single band for a series of related compounds. Others may discuss some of the infrared bands of a given compound in great detail without giving the full spectrum of the compound. Such fragmentary reports are often excluded from spectra compilations and the valuable information they contain may be lost to the researcher unless he is willing to undertake an extensive and careful literature search. In a handbook indexed by band position, the inclusion of single bands—provided they are reported with the required accuracy—presents no problem. The information and the original literature citation are then available to the reader by a simple check of the molecular formula index.

But this is of course only one of the ways in which the Handbook can be used. Others include the identification of unknown compounds by inspection in the Handbook of the regions in which strong bands are observed in the unknown spectrum. An exact identification can be made if several coincidences are found, or the Handbook entries may suggest a general formula.

The assignment of vibrations for a known compound can also be facilitated by comparing the observed spectrum with assignments in the Handbook.

Now that the Infrared Band Handbook encompasses three volumes, the question suggests itself whether the compilation of absorption bands will have to continue in perpetuity for the work to attain total effectiveness. Many spectroscopists today feel that that is not the case but that a finite number of spectra of representative compounds would yield nearly all the bands required

for the identification of nearly all conceivable compounds. We cannot be certain today exactly what that number of spectra will be, but one group of workers engaged in the compilation of spectra in a different form has suggested that 15,000 compounds would be sufficient. Presumably, the spectrum of any compound not in this set would contain a sufficient number of absorption bands that coincide with bands in the collection so that it can still be identified. If this concept is correct, we can foresee that the Infrared Band Handbook series will eventually be terminated as a definitive collection in a limited number of volumes.

In the meantime, in grateful acknowledgment of the enthusiastic reception afforded the first two volumes in the series, I shall continue with the compilation of the most recent and representative data available in the literature.

Buffalo, New York

Herman A. Szymanski

EXPLANATION

In this volume, Greek letter symbols rather than descriptive terms have been used to characterize the vibration assignments. These symbols have the following significance:

ν_γ	=	out-of-plane stretch
ν_β	=	in-plane stretch
ν_{as}	=	asymmetric stretch
ν_s	=	symmetric stretch
δ_{as}	=	asymmetic bend
δ_s	=	symmetric bend
δ'	=	deformation (bend, twist, or rock)
ω	=	wag
r	=	rock
r_β	=	in-plane rock
r_γ	=	out-of-plane rock
τ	=	torsion } usually
t	=	twist } equivalent
β	=	in-plane bend
γ	=	out-of-plane bend

The following additions have been made to the Intensity and Physical State Codes:

Intensity Code
D = doublet
T = triplet

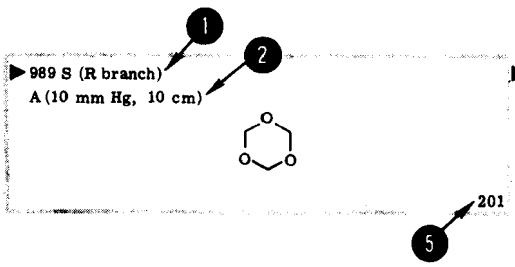
Physical State Code
R = NaCl disk

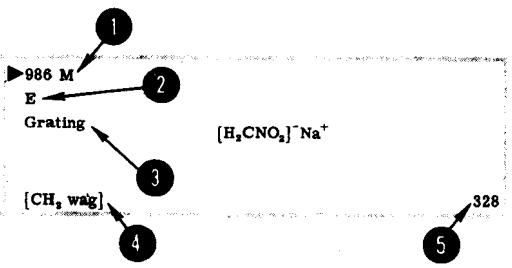
EXPLANATION

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).





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 page 247.

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.)

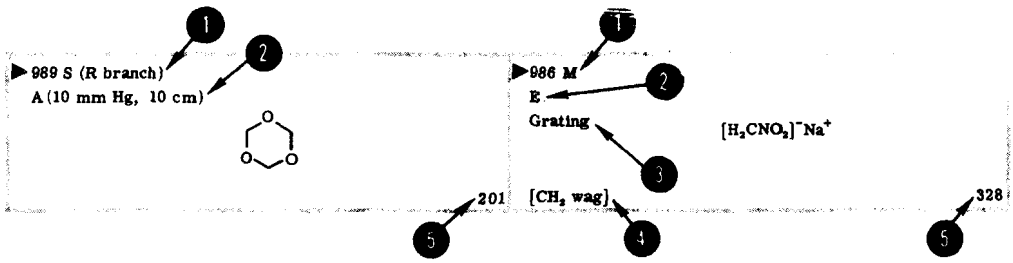
A = Vapor or gaseous state (followed by the pressure and path length, where pertinent)
B = Sample run as a liquid (followed by the cell thickness, in millimeters, where pertinent)
C = Solid, powder
D = Solid, film
E = Nujol oil
F = Fluorocarbon oil
G = KBr disk
H = Solution – solvent not specified
I = 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 isomèrisée 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 au page 247.

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 differentes longueurs de traces et/ou des concentrations differentes 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.)

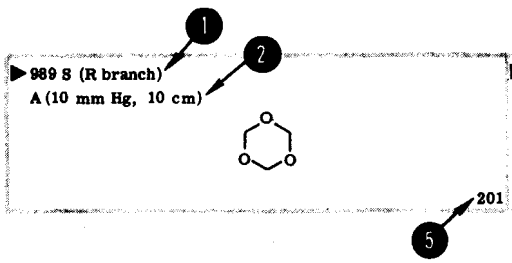
A = Vapeur ou état gazeux (suivi de la pression et la longueur du trace, là où c'est à propos)
B = Echantillon éprouvé en tant que liquide (suivi de l'épaisseur de la cellule, en millimètres, là où c'est à propos)
C = Solid, en poudre
D = Solide, pellicule
E = Huile de Nujol
F = Huile de fluorocarbone
G = Disque KBr
H = Solution—solvant non specifié
I = Etat solide—méthode non specifié
K = Ensachement polyéthylène
M = Mélange hexachlorobutadiene
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

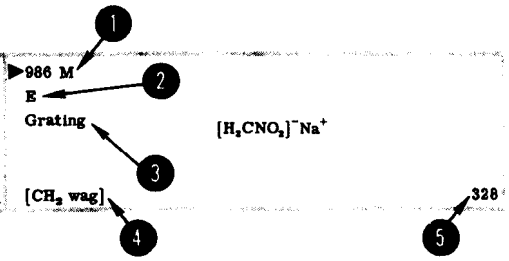
ПОЯСНЕНИЯ

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, както: 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. 247.

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°.)

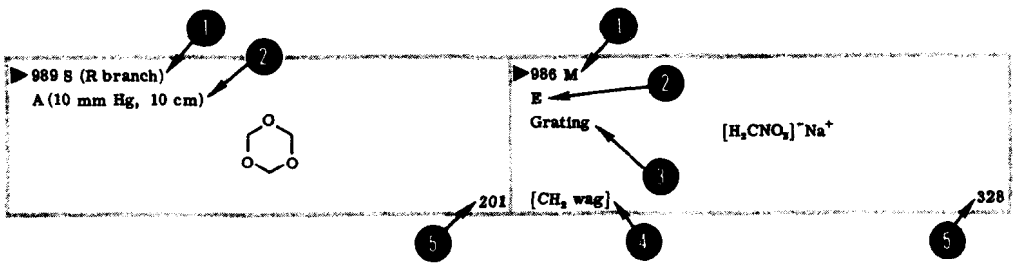
A = Паро- или газообразное состояние (с указанием давления и длины пробега там, где это существенно)
B = Проба в жидком состоянии (с указанием толщины ячейки в миллиметрах там, где это существенно)
C = Твердое тело, порошок
D = Твердое тело, пленка
E = Масло Нюжоль
F = Фтороуглеводородное масло
G = Диск KBr
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 KCl
Q = Диск KI

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 zugeteilt worden war—diese kann entweder der ursprünglichen oder der isomerischen 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. 247.

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

INFRARED ABSORPTION BANDS

CONTENTS

▶ 4240 VW
G

KCNO

2002

▶ 4115 VW
G

KCNO

2002

▶ 3860 W
B
Filter-Grating

$(CH_3)_2SO_2$

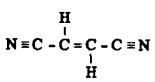
510

▶ 3857 Sh
A

C_3O_2

1019

▶ 3856 W
D
Grating



(trans)

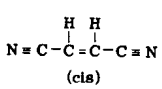
517

▶ 3849 M
A

C_3O_2

1019

▶ 3830 W
B
Grating



(cis)

517

▶ 3775 M
D(100°K)
Grating

C_3O_2

1019

▶ 3767 W
B
Filter-Grating

$(CH_3)_2SO_2$

510

▶ 3754 S
A

C_3O_2

1019

▶ 3680 VW
B

1008

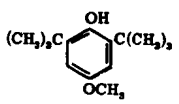
▶ 3680 VW
B

1008

▶ 3670 VW
B

1008

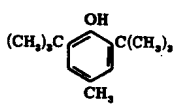
▶ 3651
$CCl_4[3\times10^{-3}M]$
Prism-Grating



[ν(OH)]

523

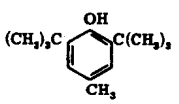
▶ 3650
$CCl_4[3\times10^{-3}M]$
Prism-Grating



[ν(OH)]

523

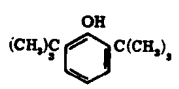
▶ 3650
CCl_4
Prism-Grating



[ν(OH)]

524

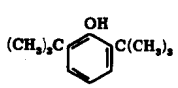
▶ 3648
CCl_4
Prism-Grating



[ν(OH)]

524

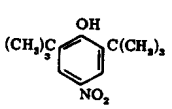
▶ 3648
$CCl_4[3\times10^{-3}M]$
Prism-Grating



[ν(OH)]

523

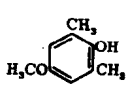
▶ 3627
$CCl_4[3\times10^{-3}M]$
Prism-Grating



[ν(OH)]

523

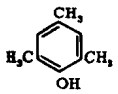
▶ 3624
$CCl_4[3\times10^{-3}M]$
Prism-Grating



[ν(OH)]

523

▶ 3622
CCl_4[3×10^{-5}M]
Prism-Grating

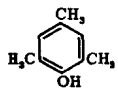


[ν(OH)] 523

▶ 3612
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3622
CCl_4
Prism-Grating



[ν(OH)] 524

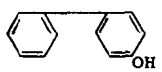
▶ 3612
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3621
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3610
CCl_4
Prism-Grating



[ν(OH)] 524

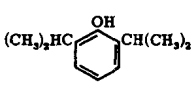
▶ 3621
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3610 VW

1008

▶ 3619
CCl_4
Prism-Grating



[ν(OH)] 524

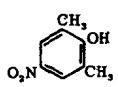
▶ 3610 M
B

1018

▶ 3618
CCl_4[3×10^{-3}M]
Prism-Grating

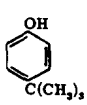
[ν(OH)] 523

▶ 3606
CCl_4[3×10^{-4}M]
Prism-Grating



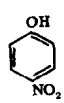
[ν(OH)] 523

▶ 3614
CCl_4
Prism-Grating



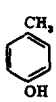
[ν(OH)] 524

▶ 3595
CCl_4[1×10^{-3}M]
Prism-Grating



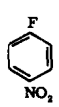
[ν(OH)] 523

▶ 3614
CCl_4
Prism-Grating



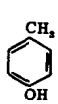
[ν(OH)] 524

▶ 3595 VW
B



1008

▶ 3614
CCl_4[3×10^{-5}M]
Prism-Grating



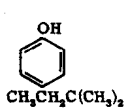
[ν(OH)] 523

▶ 3595 W
A
Grating

CF_3COCl

501

▶ 3613
CCl_4
Prism-Grating



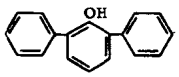
[ν(OH)] 524

▶ 3574
D
Grating

CF_3COCl

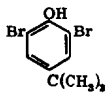
501

▶ 3555
CCl_4
Prism-Grating



[ν(OH)] 524

▶ 3521
CCl_4
Prism-Grating



[ν(OH)] 524

▶ 3549
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3520
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3542
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3520
CCl_4[very dilute]
Grating

[ν(OH)] 507

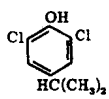
▶ 3542
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3519
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3541
CCl_4
Prism-Grating



[ν(OH)] 524

▶ 3518
CCl_4[dilute]

[$\nu_{as}(NH_2)$] 525

▶ 3538
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3517
CCl_4
Prism-Grating

[ν(OH)] 524

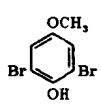
▶ 3538
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3517
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3530
CCl_4[3×10^{-3}M]
Prism-Grating



[ν(OH)] 523

▶ 3510 S
G

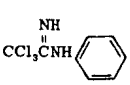
$CuSeO_3$

1005

▶ 3522
CCl_4
Prism-Grating

[ν(OH)] 524

▶ 3509
CCl_4[very dilute]
Grating

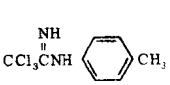


[$\nu_{as}(NH_2)$] 507

▶ 3522
CCl_4[3×10^{-3}M]
Prism-Grating

[ν(OH)] 523

▶ 3508
CCl_4[very dilute]
Grating

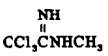


[$\nu_{as}(NH_2)$] 507

▶ 3506
CCl_4[very dilute]
Grating

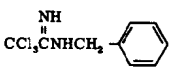
[$\nu_{as}(NH_2)$]
507

▶ 3506
CCl_4[very dilute]



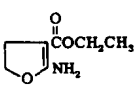
[$\nu_{as}(NH_2)$]
507

▶ 3505
CCl_4[very dilute]
Grating



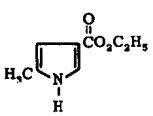
[$\nu_{as}(NH_2)$]
507

▶ 3500
$CHCl_3$



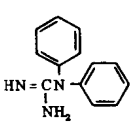
[$\nu(NH_2)$]
2000

▶ 3500
CCl_4



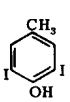
[ν(N-H)]
2001

▶ 3499
CCl_4[very dilute]
Grating



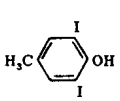
[$\nu_{as}(NH_2)$]
507

▶ 3498
CCl_4[3×10^{-3} M]
Prism-Grating



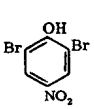
[ν(OH)]
523

▶ 3497
CCl_4
Prism-Grating



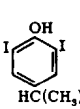
[ν(OH)]
524

▶ 3496
CCl_4[3×10^{-3} M]
Prism-Grating



[ν(OH)]
523

▶ 3495
CCl_4
Prism-Grating



[ν(OH)]
524

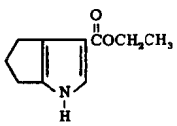
▶ 3491
CCl_4
Prism-Grating

[ν(OH)]
524

▶ 3491
CCl_4[3×10^{-3} M]
Prism-Grating

[ν(OH)]
523

▶ 3485
$CHCl_3$

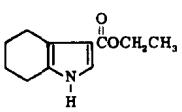


[ν(N-H)]
2001

▶ 3478 WSh
B
Filter-Grating

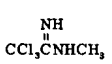
510

▶ 3475
$CHCl_3$



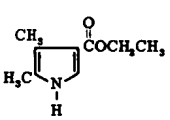
[ν(N-H)]
2001

▶ 3471
CCl_4[very dilute]



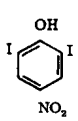
[ν(NH)]
507

▶ 3470
$CHCl_3$



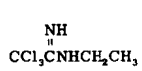
[ν(NH)]
2001

▶ 3468
CCl_4[3×10^{-3} M]
Prism-Grating



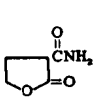
[ν(OH)]
523

▶ 3467
CCl_4[very dilute]
Grating



[ν(NH)]
507

▶ 3465
$CHCl_3$



[$\nu(NH_2)$]
518