INTERNATIONAL UNION
OF PURE AND APPLIED CHEMISTRY
COMMISSION ON
MOLECULAR STRUCTURE AND SPECTROSCOPY

TABLES OF WAVENUMBERS FOR THE CALIBRATION OF INFRA-RED SPECTROMETERS

I. TABLES FOR THE CALIBRATION OF GRATING SPECTROMETERS IN THE RANGE 4300–600 cm^{-1}

INTRODUCTION

In the past five years, the number of grating infra-red spectrometers has greatly increased. Most of the recent instruments operate mainly in the range 4000–600 cm^{-1} and have a limit of resolution between 0·1 and 1 cm^{-1}. Often, these spectrometers are not equipped for precise wavelength determination by measurement of the grating angle, and for them it is necessary, and for the others which *are* so equipped it is desirable, to have standard wavenumbers for calibration.

The precision with which a wavelength or wavenumber can be measured improves with better resolution. For a given instrument this precision can be seriously affected by mechanical instability, temperature variation and other non-spectroscopic factors. However, if it is limited only by the experimenter's ability to locate the maximum of a sharp absorption line the shape of which is determined by the slit function of an energy-limited spectrometer, the precision is likely to be from one-fifth to one-tenth of the achievable resolution. That is, a spectrometer whose best resolution is about 0·3 cm^{-1} will be capable of a wavenumber precision of about ± 0·03–0·06 cm^{-1}. Thus the wavenumber standards to be used for the calibration of such spectrometers should have an absolute accuracy of ± 0·03 cm^{-1} or better.

Until quite recently no measurements in the infra-red from 2000 to 600 cm^{-1}, and very few from 4000 to 2000 cm^{-1}, were of this accuracy. It was therefore necessary to use higher orders of atomic emission lines for calibration, a procedure capable of high accuracy but having many pitfalls and inconveniences. With the extension of precise measurement to lower wavenumbers by several laboratories in various countries, it has become possible to compare the wavenumber values for molecular absorption bands determined with respect to different standards of higher-order emission and absorption lines in different laboratories, and thereby to assess the absolute accuracy of these measurements.

In view of the urgent need for wavenumber standards in the infra-red, the Commission on Molecular Spectroscopy has made such an assessment of existing data (including certain measurements carried out specifically for the Commission), and is presenting the results without delay in the following tables of *provisional wavenumbers*. The Commission does not regard the data in these tables as *standard*, since they have not met tests usually required of standard wavelengths in the visible region. Moreover, the accuracy of the molecular data will undoubtedly be improved in the next few years. However, until more powerful spectrometers for the region below 2000 cm^{-1} are built and a broader effort can be made in the measurement, evaluation and tabulation of standard wavenumbers, these tables are believed to represent very nearly the best that can be done with existing data. They are considered to be reliable to ±0·03 cm^{-1} or better, except in those cases where for one reason or another as stated, the values are less accurate.

SOURCES OF DATA FOR THE TABLES

The molecular data in these tables are presented as wavenumbers in cm^{-1} *in vacuo*. The Commission believes that there are important reasons for the use of wavenumbers rather than wavelengths in infra-red spectroscopy. The wavenumber values, being values calculated from wavelengths measured in air, are of course dependent in accuracy on the accuracy with which the refractive index of air is known. Since the latter accuracy is considerably better than that of standard infra-red wavelengths, the accuracy of the calculated wavenumbers is not inferior to that of the observed wavelengths.

Standard infra-red wavelengths of atomic emission spectra are essential in the determination of wavenumber values of molecular absorption lines. These wavelengths may also prove useful for calibration of grating spectrometers in the range 10,000–4,000 cm^{-1}. For this reason tables of standard wavelengths in air in the range 1–2·5 μ and their calculated wavenumbers in cm^{-1} *in vacuo* are included herewith. A complete table for conversion of wavelengths in air to wavenumbers is also given for the range 1–20 μ (10,000–500 cm^{-1}).

STANDARD WAVELENGTHS AND WAVENUMBERS OF ATOMIC EMISSION LINES

In 1907 the International Union for Co-operation in Solar Research adopted[1] as the primary standard of wavelength the red cadmium line with the wavelength specified as 6438·4696 Å for standard air. Recently, the orange line of krypton-86 has been measured near the triple point of nitrogen in several laboratories, and the wavelength has been reported[2] to be 6057·8021 Å for vacuum, 6056·1252 Å for standard air, relative to the red line of cadmium. The krypton-86 line was adopted as the primary standard for all length measurements by the General Conference on Weights and Measures, meeting at Paris in October, 1960.

In 1950 Meggers and Westfall[3] devised a simple tube containing mercury-198 which emits sharp lines when the vapour is excited by an electrode-less, high-frequency discharge. Meggers and others have measured the wavelength of the green mercury line with very high precision and the accepted wavelength is 5460·7532 Å for standard air[4]. There are several features which make the mercury-198 lamp well suited for laboratory use. The lamp is rugged, of long life and easy to operate, and the green line is intense and readily isolated. For these reasons the green line of mercury-198 is recommended as a laboratory standard for all spectroscopic wavelength measurements. A very small pressure shift which has been observed in the position of this line is produced by the action of the carrier gas, but in ordinary uses this effect need not be taken into consideration. The mercury-198 lamp with the high-frequency discharge equipment can be obtained from commercial sources.

Many atomic lines have been measured with high precision by the use of a Fabry-Perot interferometer, and these lines, which fall mainly in the visible and ultra-violet regions, can be used in higher orders for calibrating infra-red spectrometers. The iron spectrum has been used as a secondary standard for many years, and by 1955 precise measurements were reported[5] from several laboratories on 575 iron lines between 2500 and 9400 Å. In 1957 Stanley and Meggers[6] reported the wavelengths of 103 iron lines measured with a Fabry-Perot interferometer in the range from 2900 to 4100 Å. In view of the wide availability of tables of wavelengths of the iron lines, they will not be included here.

The spectra of the rare gases are rich in lines in the visible and near infra-red regions. A large number of lines in these gases have been measured with a Fabry-Perot interferometer by Meggers and Humphreys[7]. Paul and Humphreys[8] have extended the interferometric measurements of the spectrum of neon, argon, and krypton to 2 μ. Recently Burns, Adams and Longwell[9] have made many determinations of the wavelengths of the lines of neon. The wavelengths listed in *Table A* are mainly from their work, except for some lines which are from the references 7–11. *Table B* gives additional neon wavelengths which have been calculated by the combination principle[11]. Also, Burns and Adams[10] have made many measurements of the wavelengths of the lines of argon. Their values are listed in *Table C* with some additional lines by other workers.

Tables C, D and E list the intense lines of argon, krypton and xenon with wavelengths greater than 7000 Å. The listed values are experimentally determined except in a few cases where calculated values are added. By the use of the combination principle the wavelengths of a number of lines entered in the tables have been calculated. The agreement with the experimental values is excellent. The calculated values are given in references 5, 10 and 11. Additional lines with wavelengths less than 5800 Å can be found in the paper of Meggers and Humphreys[7]. Rao, Coburn, Garing, Rossman and Nielsen[12] have used the higher orders of the visible lines of neon for calibration in the region from 10 to 20 μ. As is well known, the intercomparison of higher orders in some gratings has led in the past to errors on account of imperfections of the optical properties of the grating. However, with modern gratings of high quality, the use of higher orders is quantitatively satisfactory.

Several lines of mercury-198 have been measured with a Fabry-Perot interferometer in the infra-red region by Paul and Humphreys[8], Rank and co-workers[13], and Peck[14]. The results reported in these papers are listed in *Table F*.

There are a number of lines in the infra-red region which have been measured by a comparison spectrum but not with an interferometer. It is estimated that they are, on the average, correct to one part in 100,000 ($\sim$0·1 cm^{-1}). These lines have been reported by Plyler, Blaine, and Tidwell[15], Meggers[16], and Humphreys and Kostkowski[17]. A selected list of these lines is given in *Table G*. It should be emphasized that these lines should not be used for high precision measurement, especially in the regions where more precisely measured lines of neon, argon, krypton, xenon and mercury-198 are available. They are useful in higher orders since the uncertainty of the wavenumber is inversely proportional to the grating order.

Discharge tubes containing various gases can be obtained from several commercial suppliers. Hollow-cathode tubes containing one or more rare gases have also been designed and used for sources[12,19]. The hollow-cathode source has been used for the iron spectrum in place of the open-air arc. Stanley and Meggers[6] have shown that a tube containing $FeBr_3$ and helium at 2 mm pressure emits very sharp iron lines when excited by a high frequency generator. Relatively intense spectra of the rare gases can be obtained by the use of a low pressure electrode-less tube excited by a microwave source.

Table A. Intense emission lines of neon, 5800–9700 Å, experimentally measured

λ_{air} (Å)	ν (cm^{-1})	λ_{air} (Å)	ν (cm^{-1})
5852·4878	17082·016	8128·9077	12298·394
5881·8950	16996·613	8136·4061	12287·060
5913·633	16905·394	8248·6812	12119·819
5944·8342	16816·669	8259·3795	12104·120
5965·474	16758·486	8266·0788	12094·310
5974·628	16732·809	8267·1166	12092·792
5975·5340	16730·272	8300·3248	12044·411
5987·9069	16695·701	8365·7464	11950·222
6029·9971	16579·165	8377·6062	11933·305
6074·3377	16458·144	8417·1614	11877·227
6096·1630	16399·221	8418·4265	11875·441
6128·4498	16312·826	8463·3569	11812·397
6143·0623	16274·023	8484·4424	11783·042
6163·5939	16219·8123	8495·3591	11767·900
6182·146	16171·138	8544·6952	11699·954
6217·2813	16080·752	8571·3535	11663·595
6266·4950	15953·471	8591·2583	11636·542
6304·7893	15856·573	8634·6472	11578·068
6334·4279	15782·381	8647·0400	11561·475
6382·9914	15662·306	8654·3837	11551·664
6402·2460	15615·202	8655·5206	11550·148
6506·5279	15364·935	8679·4898	11518·250
6532·8834	15302·949	8681·9216	11515·024
6598·9529	15149·735	8704·1132	11485·671
6652·0925	15028·714	8771·6592	11397·222
6678·2764	14969·790	8780·6223	11385·588
6717·430	14883·394	8783·7539	11381·528
6929·4672	14427·144	8830·9078	11320·756
7024·0500	14232·876	8853·8669	11291·399
7032·4128	14215·950	8865·3057	11276·831
7059·1079	14162·191	8865·7562	11276·257
7173·9380	13935·505	8919·4987	11208·314
7245·1665	13798·503	9486·680	10538·205
7438·8981	13439·150	9534·164	10485·721
7488·8712	13349·472	9665·424	10343·321
7535·7739	13266·384		
7544·0439	13251·841		
7943·1805	12585·954		
8082·4576	12369·074		
8118·5495	12314·085		

Table B. Additional intense neon lines calculated from energy levels derived from interferometric measurements

λ_{air} (Å)	ν (cm^{-1})	λ_{air} (Å)	ν (cm^{-1})
8301·557	12042·623	19573·664	5107·511
8376·359	11935·081	19577·045	5106·629
8778·732	11388·039	20350·153	4912·625
9148·670	10927·552	21708·060	4605·327
9201·757	10864·509	22247·379	4493·685
9220·057	10842·948	22428·125	4457·471
9221·578	10841·156	22466·845	4449·789
9226·690	10835·150	22530·281	4437·261
9275·517	10778·113	22661·688	4411·530
9300·852	10748·754	23260·164	4398·023
9310·584	10737·519	23565·267	4242·376
9313·971	10733·614	23636·375	4229·613
9326·504	10719·190	23701·698	4217·956
9373·308	10665·666	23707·651	4216·897
9425·379	10606·743	23709·061	4216·646
9433·005	10598·168	23978·161	4169·324
9459·209	10568·809	24098·598	4148·487
9547·406	10471·177	24161·476	4137·691
10562·408	9464·945	24218·996	4127·864
11143·018	8971·773	24364·937	4103·139
11177·531	8944·070	24371·637	4102·011
11390·440	8776·889	24447·900	4089·215
11525·016	8674·403	24459·451	4087·284
11536·346	8665·883	24459·714	4087·240
11688·008	8553·437	24776·510	4034·980
11789·041	8480·133	24903·795	4014·357
11789·895	8479·519	24928·932	4010·309
12066·341	8285·249	25161·733	3973·205
12459·386	8023·883	25524·212	3916·780
12595·001	7937·486		
12689·199	7878·563		
12769·534	7828·998		
12912·023	7742·602		
13219·251	7562·657		
17161·938	5825·257		

Table C. Intense emission lines of argon, 6900–17,000 Å

λ_{air} (Å)	ν (cm^{-1})	λ_{air} (Å)	ν (cm^{-1})
6965·4304	14352·656	11488·108*	8702·271
7030·262	14220·300	11668·708	8567·584
7067·2175	14145·940	12112·323	8253·796
7147·0408	13987·950	12139·735	8235·158
7272·9349	13745·821	12343·390	8099·286
7372·117	13560·889	12402·826	8060·473
7383·9800	13539·103	12439·318	8036·827
7503·8676	13322·793	12456·112	8025·991
7514·6514	13303·674	12487·661	8005·715
7635·1053	13093·792	12702·278	7870·450
7723·7599	12943·500	12733·414	7851·206
7724·2064	12942·752	12802·737	7808·694
7891·075	12669·060	12933·190	7729·930
7948·1755	12578·045	12956·656	7715·930
8006·1566	12486·953	13008·260	7685·321
8014·7853	12473·511	13213·989	7565·668
8053·307	12413·845	13228·103	7557·596
8103·6920	12336·663	13230·891	7556·003
8115·3109	12319·000	13272·632	7532·241
8264·5209	12096·590	13313·206	7509·285
8408·2094	11889·872	13367·109	7479·004
8424·6473	11866·673	13406·586	7456·981
8521·4407	11731·881	13504·188	7403·086
8667·9430	11533·594	13599·333	7351·292
9122·9660	10958·340	13622·654	7338·707
9224·498	10837·724	13678·546	7308·720
9354·218	10687·432	13718·575	7287·394
9657·7841	10351·504	14093·635	7093·462
9784·5010	10217·443	15046·503	6644·247
10470·053*	9548·433	15301·879	6533·360
10478·033	9541·162	16180·017*	6178·775
10673·566	9366·374	16940·578	5901·374
10681·771	9359·180	17914·627*	5580·507
11078·867	9023·723	17914·723*	5580·477
11441·830	8737·469	25505·237*	3919·694
		25661·035*	3895·895

* Calculated values.

Table D. Intense emission lines of krypton, 7400–20,000 Å

λ_{air} (Å)	ν (cm^{-1})
7486·862	13353·053
7587·4130	13176·096
7601·5443	13151·602
7685·2460	13008·365
7694·5395	12992·654
7854·8217	12727·532
8059·5038	12404·301
8104·3642	12335·640
8112·902	12322·658
8190·0543	12206·576
8263·2398	12098·465
8281·0495	12072·446
8298·1077	12047·629
8508·8700	11749·214
8776·7490	11390·612
8928·6920	11196·774
9751·759	10251·749
11819·374	8458·370
13177·403	7586·674
13622·404	7338·841
13634·215	7332·484
14426·786	6929·657
14734·440	6784·966
15239·608	6560·056
15334·966	6519·264
16785·127	5956·028
16853·490	5931·869
16890·444	5918·891
16896·744	5916·684
16935·799	5903·040
18002·222	5553·353
18167·320	5502·887

Table E. Intense emission lines of xenon, 7000–10,000 Å

λ_{air} (Å)	ν (cm^{-1})
7119·598	14041·866
7285·301	13722·488
7316·272	13664·398
7321·452	13654·731
7386·003	13535·395
7393·793	13521·134
7584·680	13180·843
7642·025	13081·936
7802·651	12812·631
7881·320	12684·741
7887·3898	12674·979
7967·342	12547·786
8057·258	12407·758
8061·339	12401·477
8206·336	12182·358
8231·6336	12144·919
8280·1162	12073·807
8346·8217	11977·317
8409·1894	11888·486
8739·372	11439·328
8819·411	11335·512
8952·2506	11167·309
9045·4460	11052·253
9162·6520	10910·876
9513·377	10508·631
9799·697	10201·600
9923·198	10074·635

Table F. Intense emission lines of ^{198}Hg, 10,000–18,000 Å

λ_{air} (Å)	ν (cm^{-1})
10139·793	9859·432
11287·406	8857·006
12071·604	8281·568
13570·573	7366·870
13673·398	7311·471
15295·976	6535·882
16920·659	5908·322
16942·474	5900·714
17073·120	5855·561
17109·893	5842·976

Table G. Additional emission lines of argon, neon, krypton, xenon, and Hg, 7600–40,000 Å, accurate to ±0·10 cm^{-1} but not measured with an interferometer

Gas	λ_{air} (Å)	ν (cm^{-1})	*Gas*	λ_{air} (Å)	ν (cm^{-1})
Xe	7643·91	13078·71	Ne	18591·12	5377·44
Xe	8648·54	11559·47	Ne	18597·30	5375·66
Xe	8862·32	11280·63	Xe	18788·13	5321·06
Xe	8908·73	11221·87	A	19817·54	5044·66
Xe	8987·57	11123·43	Kr	20209·87	4946·73
Xe	9374·76	10664·01	Xe	20262·28	4933·93
Kr	10593·01	9437·60	Kr	20423·93	4894·88
Ne	10620·70	9413·00	A	20616·21	4849·23
Xe	10706·78	9337·32	A	20986·10	4763·76
Xe	10758·86	9292·12	Kr	21165·14	4723·46
Ne	10798·06	9258·39	Xe	21470·00*	4656·39
Xe	10838·34	9223·98	A	21534·16	4642·52
Ne	10844·49	9218·75	Kr	21902·51	4564·44
Kr	10874·92	9192·95	A	22077·20	4528·32
Xe	10895·32	9175·74	Kr	22485·52	4446·09
Xe	11085·25	9018·53	Hg	22493·28	4444·56
Xe	11127·20	8984·53	Xe	23193·28*	4310·42
Kr	11257·74	8880·35	Hg	23253·07	4299·33
Ne	11409·24	8762·43	Kr	23340·07	4283·31
Kr	11457·52	8725·50	Ne	23372·81	4277·31
Ne	11522·82	8676·06	Kr	23502·55	4253·70
Xe	12623·36	7919·65	A	23845·13	4192·58
Xe	13657·22	7320·13	Kr	24260·54	4120·80
Kr	13738·94	7276·59	Kr	24292·16	4115·43
Kr	13883·15	7201·01	Xe	24824·63*	4027·14
Kr	13924·11	7179·82	A	25125·08	3979·00
Xe	14241·23	7019·95	Kr	25233·77	3961·86
Kr	14347·69	6967·86	Xe	26268·95*	3805·74
Xe	14732·88	6785·68	Xe	26510·96*	3771·00
Xe	15418·12	6484·10	Hg	32148·06	3109·76
Xe	17325·79	5770·17	Hg	36303·03	2753·84
Kr	17367·80	5756·21	Hg	39283·61	2544·90
Ne	18082·71	5528·63			
Ne	18276·59	5469·99			
Ne	18282·58	5468·20			
Ne	18304·00	5461·79			
Ne	18385·17	5437·68			
Ne	18390·10	5436·22			
Ne	18403·16	5432·37			
Ne	18422·43	5426·68			

* Calculated values.

In the measurement of the higher orders of atomic lines in the infra-red region, the intensities observed will vary with the source and the method of excitation. However, the greatest variation of intensity arises from the characteristics of the grating used. The first-order spectrum may be weak and the higher orders intense, or some high orders may be very weak. The intensity of a line may be misleading and the position or wavelength should be the key to identification. An example of the changes in intensity with the order in which the gratings are used is shown in *Figures A* and *B*. In *Figure A*

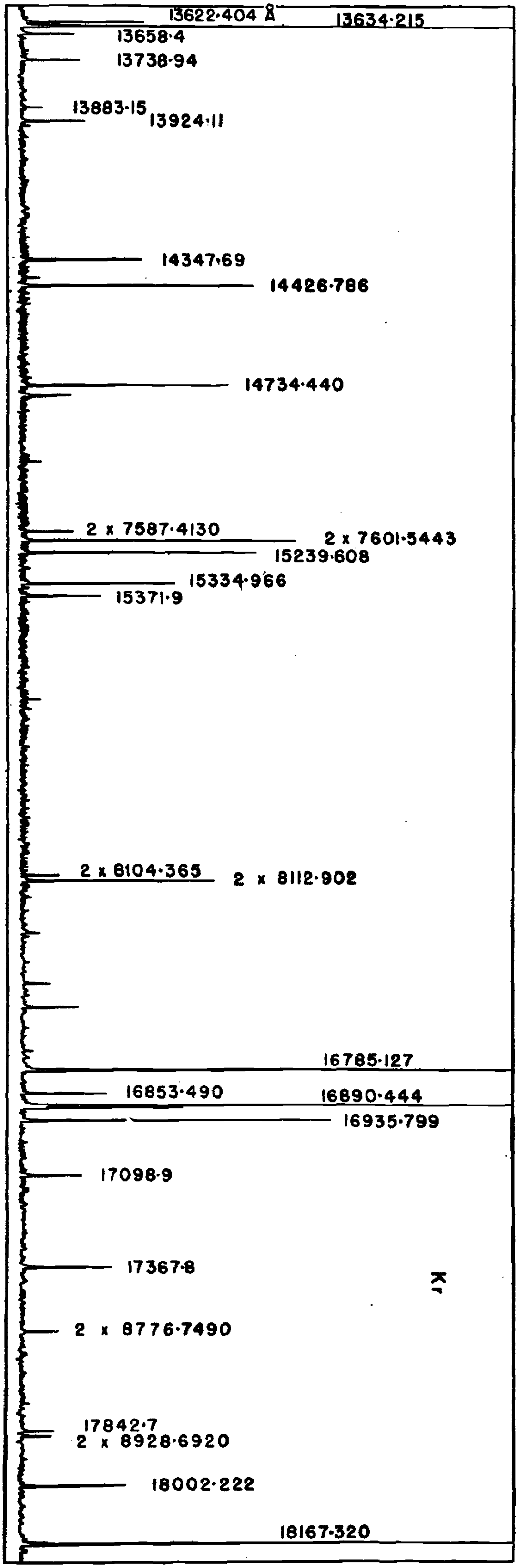


Figure A. The first- and second-order lines of krypton in the region from 1·36 to 1·82 μ as observed with a grating of 15,000 lines/in.

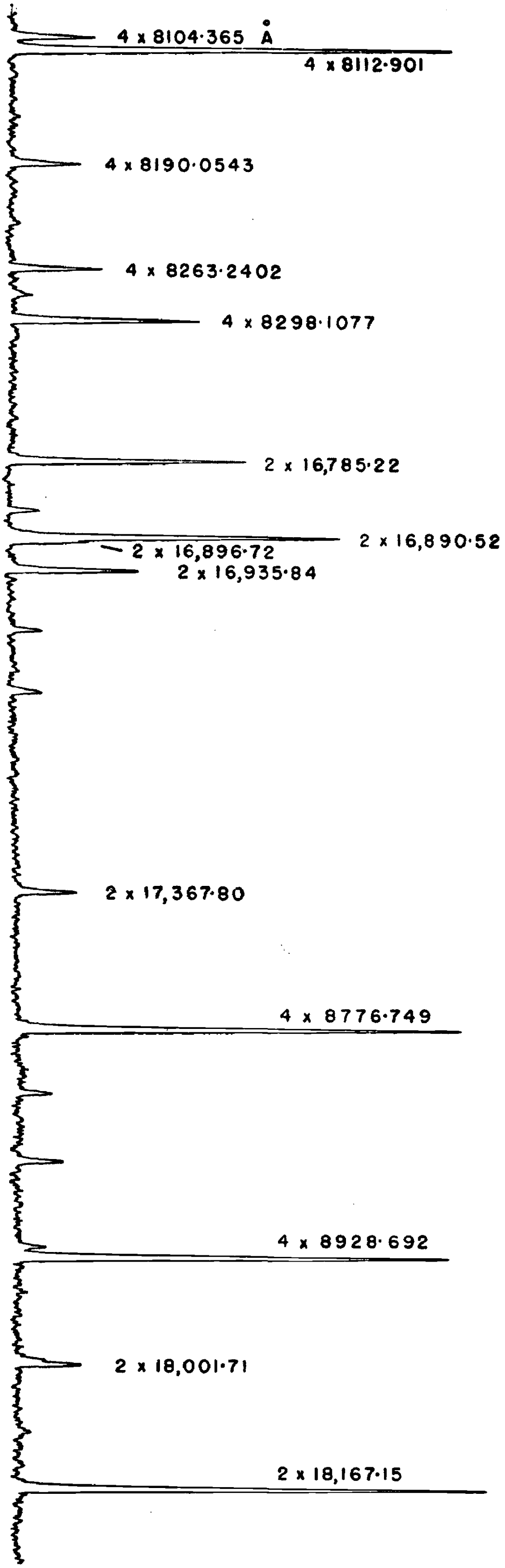


Figure B. The second- and fourth-order lines of krypton in the region from 3·2 to 3·7 μ as observed with a 7500 lines/in. grating

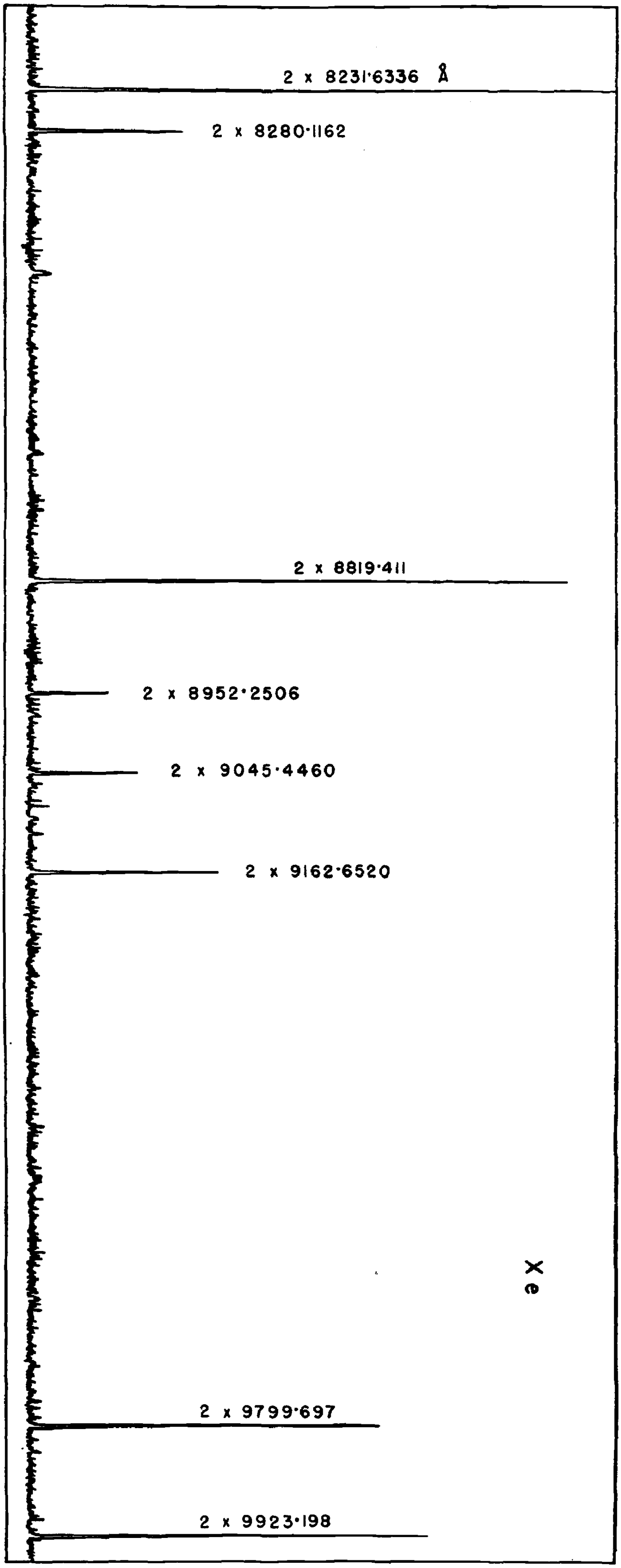


Figure C. The second-order lines of xenon in the region from 1·6 to 2 μ as observed with a 10,000 lines/in. grating some first- and second-order lines of krypton are recorded in the region from 1·36 to 1·82 μ with a grating ruled with 15,000 lines/in. In *Figure B* some of the same lines are recorded in the second- and fourth-orders of a grating having 7500 lines/in. A comparison of these two figures shows that the higher order lines are less intense with the grating of 15,000 lines/in. than with the one having 7500 lines/in., the influence of the grating being especially noticeable in the observed intensities of the higher orders of lines from 7500 to 9000 Å. A part of the xenon spectrum is shown in *Figure C*. There are no intense first-order lines in the region from 1·6 to 2 μ but a number of second-order lines are observed.

REFRACTIVE INDICES OF AIR

Wavelengths of lines have usually been measured in air and in order to compare work carried out in different laboratories final results are reduced to standard air. Standard air is defined as dry air at a pressure of 760 mm Hg and at a temperature of 15°C, having 0·03 per cent CO_2 by volume. These conditions are not usually fulfilled in the laboratory, and a reduction of the data taken under conditions differing from those of standard air must be made. Penndorf[20] has given an equation for the influence of pressure and temperature on the index of refraction of air, which is:

$$(n - 1) = (n_s - 1)\,\frac{1 + \alpha t_s}{1 + \alpha t}\,\frac{P}{P_s}$$

where $t_s = 15°C$, t = temperature in °C of the air surrounding the dispersing element, P = atmospheric pressure in laboratory in mm, P_s = 760 mm, n_s is the index of refraction of standard air and n is the index of refraction at $t°$ and P mm. The optical temperature coefficient, denoted by α, has the approximate value 0·00366. Small changes in CO_2 content and the humidity of the air do not appear to change the indices of air appreciably. No extensive tables have been provided for these corrections and they are usually neglected. However, in the future when experimental values of the indices of refraction are determined in the neighbourhood of 2·7, 4·3 and 6·2 μ, a detectable effect may be observed for changes in the amount of water vapour and CO_2 in the air.

The influence of temperature on the refractive index of air is appreciable, and temperature corrections must be made. Penndorf[20] has calculated a table which gives the value of the indices of refraction of air from 0·2 to 20·0 μ for temperatures ranging from −30°C to +30°C. For example, at 15°C, $(n - 1) \times 10^8$ is 27,277 and at 30°C, is 25,925, for 3 μ radiation. If the air temperature were 30°C and the refractive index of air at 15°C were used for reducing the data to cm^{-1}, an error of 0·045 cm^{-1} would result.

For many years Kayser's "Tabellen der Schwingungszahlen" have served as a ready means for reducing wavelengths in air to cm^{-1} in vacuum. These tables did not extend past 1·0 μ, but Babcock[21] demonstrated how they could be used further in the infra-red region, and gave a table of corrections.

In recent years new measurements on the refractive index of air have shown that the formula used by Kayser for the calculation of his table was not

Table H. Wavelength-to-wavenumber conversion tables and refractive index of standard air, 2–20 μ

Wavelength (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n-1)$ $\times 10^9$ *for* 15°C	*Wavelength* (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n-1)$ $\times 10^9$ *for* 15°C
2·00000	4998·636	272984	2·90000	3447·336	272782
·02	4949·144	976	·92	23·724	779
·04	4900·623	969	·94	00·433	777
·06	4853·044	961	·96	3377·457	774
·08	4806·380	955	·98	54·790	772
2·10000	4760·605	272948	3·00000	3332·424	272770
·12	4715·694	941	·02	10·355	767
·14	4671·622	935	·04	3288·577	765
·16	4628·367	929	·06	67·083	763
·18	4585·904	923	·08	45·868	761
2·20000	4544·214	272917	3·10000	3224·927	272759
·22	4503·276	911	·12	04·254	757
·24	4463·068	905	·14	3183·845	755
·26	4423·572	900	·16	63·694	753
·28	4384·768	895	·18	43·797	751
2·30000	4346·640	272890	3·20000	3124·148	272749
·32	4309·169	885	·22	04·743	747
·34	4272·339	880	·24	3085·578	745
·36	36·132	875	·26	66·648	744
·38	00·535	870	·28	47·949	742
2·40000	4165·530	272866	3·30000	3029·477	272740
·42	4131·104	862	·32	11·227	738
·44	4097·243	857	·34	2993·196	737
·46	63·932	853	·36	75·379	735
·48	31·158	849	·38	57·773	734
2·50000	3998·909	272845	3·40000	2940·375	272732
·52	67·172	841	·42	23·179	730
·54	35·934	837	·44	06·184	729
·56	05·185	834	·46	2889·385	727
·58	3874·912	830	·48	72·780	726
2·60000	3845·105	272826	3·50000	2856·364	272724
·62	15·753	823	·52	40·135	723
·64	3786·846	820	·54	24·089	722
·66	58·373	816	·56	08·223	720
·68	30·326	813	·58	2792·535	719
2·70000	3702·694	272810	3·60000	2777·021	272718
·72	3675·468	807	·62	61·678	716
·74	48·640	804	·64	46·504	715
·76	22·200	801	·66	31·496	714
·78	3596·141	798	·68	16·651	712
2·80000	3570·455	272795	3·70000	2701·966	272711
·82	45·132	792	·72	2687·439	710
·84	20·167	790	·74	73·068	709
·86	3495·550	787	·76	58·849	708
·88	71·275	784	·78	44·781	707

Table H. (continued)

Wavelength (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n-1)$ $\times 10^9$ *for* 15°C	*Wavelength* (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n-1)$ $\times 10^9$ *for* 15°C
3·80000	2630·862	272705	5·00000	1999·455	272660
·82	17·087	704	·05	79·658	659
·84	03·457	703	·10	60·250	658
·86	2589·967	702	·15	41·218	657
·88	76·617	701	·20	22·553	656
3·90000	2563·404	272700	5·25000	1904·243	272655
·92	50·325	699	·30	1886·278	654
·94	37·379	698	·35	68·649	653
·96	24·564	697	·40	51·347	652
·98	11·878	696	·45	34·362	651
4·00000	2499·319	272695	5·50000	1817·686	272650
·025	83·795	694	·55	01·311	649
·050	68·463	693	·60	1785·228	648
·075	53·319	692	·65	69·429	647
·100	38·360	690	·70	53·908	646
·125	23·582	689			
·150	08·982	688	5·75000	1738·656	272645
·175	2394·557	687	·80	23·668	645
			·85	08·936	644
4·20000	2380·303	272686	·90	1694·453	643
·225	66·219	685	·95	80·214	642
·250	52·300	684			
·275	38·544	683	6·00000	1666·212	272642
·300	24·947	682	·05	52·442	641
·325	11·508	681	·10	38·897	640
·350	2298·224	680	·15	25·573	640
·375	85·091	679	·20	12·464	639
4·40000	2272·108	272678			
·425	59·271	677	6·25000	1599·564	272638
·450	46·578	677	·30	86·869	638
·475	34·028	676	·35	74·374	637
·500	21·616	675	·40	62·074	637
·525	09·342	674	·45	49·965	636
·550	2197·203	673			
·575	85·197	672	6·50000	1538·042	272635
			·55	26·301	635
4·60000	2173·321	272672	·60	14·739	634
·625	61·573	671	·65	03·350	634
·650	49·951	670	·70	1492·131	633
·675	38·454	669			
·700	27·080	669	6·75000	1481·078	272633
·725	15·825	668	·80	70·187	632
·750	04·689	667	·85	59·456	632
·775	2093·670	666	·90	48·880	631
			·95	38·457	631
4·80000	2082·765	272666			
·825	71·974	665	7·00000	1428·182	272630
·850	61·294	664	·05	18·053	630
·875	50·723	664	·10	08·067	629
·900	40·260	663	·15	1398·220	629
·925	29·903	662	·20	88·510	629
·950	19·651	662			
·975	09·502	661			

Table H. (continued)

Wavelength (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n - 1)$ $\times 10^9$ *for* 15°C	*Wavelength* (μ)	$\nu_{\text{vac.}}$ (cm^{-1})	*Index* $(n - 1)$ $\times 10^9$ *for* 15°C
7·25000	1378·934	272628	11·5000	869·328	272611
·30	69·490	628	·6	61·834	610
·35	60·173	627	·7	54·468	610
·40	50·983	627	·8	47·227	610
·45	41·916	627	·9	40·107	610
7·50000	1332·970	272626	12·0000	833·106	272610
·55	24·142	626	·1	26·221	610
·60	15·431	626	·2	19·449	609
·65	06·833	625	·3	12·787	609
·70	1298·347	625	·4	06·232	609
7·75000	1289·971	272625	12·5000	799·782	272609
·80	81·702	624	·6	93·435	609
·85	73·538	624	·7	87·187	609
·90	65·478	624	·8	81·037	608
·95	57·519	623	·9	74·983	608
8·00000	1249·659	272623	13·0000	769·021	272608
·1	34·231	622	·2	57·369	608
·2	19·180	622	·4	46·065	608
·3	04·491	621	·6	35·094	607
·4	1190·152	621	·8	24·440	607
8·50000	1176·150	272620	14·0000	714·091	272607
·6	62·474	620	·2	04·033	607
·7	49·112	619	·4	694·255	606
·8	36·054	619	·6	84·745	606
·9	23·289	618	·8	75·492	606
9·00000	1110·808	272618	15·0000	666·485	272606
·1	1098·602	618	·2	57·715	606
·2	86·660	617	·4	49·174	606
·3	74·976	617	·6	40·851	605
·4	63·540	616	·8	32·739	605
9·50000	1052·345	272616	16·0000	624·830	272605
·6	41·383	616	·2	17·116	605
·7	30·647	615	·4	09·590	605
·8	20·130	615	·6	02·245	605
·9	09·826	615	·8	595·076	604
10·0000	999·727	272614	17·0000	588·075	272604
·1	89·829	614	·2	81·237	604
·2	80·125	614	·4	74·556	604
·3	70·609	614	·6	68·027	604
·4	61·276	613	·8	61·645	604
10·5000	52·121	272614	18·0000	555·404	272604
·6	43·139	613	·2	49·301	604
·7	34·325	612	·4	43·330	604
·8	25·674	612	·6	37·488	603
·9	17·181	612	·8	31·770	603
11·0000	908·843	272612	19·0000	526·172	272603
·1	900·655	611	·2	20·691	603
·2	892·614	611	·4	15·323	603
·3	84·715	611	·6	10·065	603
·4	76·954	611	·8	04·913	603
			20·0000	499·864	272603

accurate. In 1953, Edlén[22] proposed the following relation for the indices of refraction of standard air:

$$(n_s - 1)\, 10^8 = 6432{\cdot}8 + \frac{2{,}949{,}810}{146 - \nu^2} + \frac{25{,}540}{41 - \nu^2}$$

ν is the vacuum wavenumber in μ^{-1}, that is, $\nu = 1/(\lambda$ in microns).

From Edlén's formula, Coleman, Bozman and Meggers[23] have calculated conversion tables for wavelengths in air to wavenumbers in vacuum for the region from 2000 Å to 1000 μ. These tables should be of great value in the reduction of wavelengths measured in air to cm^{-1} in vacuum. In *Table H* are given a few values quoted from Vol. 2 of the above mentioned tables for the region from 2–20 μ.

When unknown wavelengths are measured in a grating spectrometer in air with respect to standard wavelengths in a different grating order, it is of course necessary to use the index of refraction of air at the corresponding wavelengths to obtain the wavenumbers. The procedure for doing this is described on p. 555 in the section "Procedures for the Use of the Tables".

TABLES OF WAVENUMBERS OF INFRA-RED ABSORPTION LINES IN THE SPECTRA OF GASEOUS MOLECULES

It is important to distinguish between the precision of the data, which is a measure of their self-consistency, and the absolute accuracy, which measures both the self-consistency and the systematic error. For twenty years or more, infra-red data in the range 5000–500 cm^{-1} have been reported to $\pm 0{\cdot}01$ cm^{-1}, with a precision of $\pm 0{\cdot}1$ cm^{-1} or even better. It is only in the past eight or ten years that infra-red data have had a demonstrable absolute accuracy better than $\pm 0{\cdot}1$ cm^{-1}.

The first molecular measurements of accuracy approaching $\pm 0{\cdot}01$ cm^{-1} below 5000 cm^{-1} were those of Rank and co-workers[24] and Plyler, Allen and Tidwell[25]. These two groups independently measured the lines of the carbon monoxide overtone band at 4300–4100 cm^{-1} to 0·001 cm^{-1} and agreed on most of the measured lines to better than 0·01 cm^{-1}. The measurements were made in both laboratories with reference to standard atomic emission lines in higher grating orders. Since the absolute wavelengths of these emission lines are known to one part in five million or better, direct comparison of molecular absorption lines with them in overlapping orders is potentially capable of the same kind of accuracy (the procedures for comparison are discussed in the preceding sections and references there cited). The agreement ($\pm 0{\cdot}01$ cm^{-1}) between the results of the two sets of measurements on carbon monoxide, which are of comparable precision, is taken as a measure of their absolute accuracy.

The same methods had been applied by Plyler, Blaine and Connor[26] to the lines of the fundamental band of carbon monoxide at 2000–2250 cm^{-1}. These measurements have a precision of better than $\pm 0{\cdot}01$ cm^{-1}, and their absolute accuracy has been checked by Rank and co-workers[24] with the help of calculations based on the overtone band. The check indicates that the accuracy of the measurements on the fundamental is $\pm 0{\cdot}01$ cm^{-1}. A similar check has been made by Rank, Skorinko, Eastman and Wiggins[27] of the measurements by Rao, Brim and Hoffman[28] on the fundamental band of hydrogen cyanide at 800–640 cm^{-1}. Again the agreement indicates an accuracy of ±0·01 cm^{-1}, at least for lines of small J-value. The calculations and measurements of Rank and co-workers on the hydrogen cyanide fundamental (3400–3200 cm^{-1}) are stated to be accurate to one part in one million, or ±0·003 cm^{-1}.

The foregoing measurements on carbon monoxide and hydrogen cyanide probably represent the best thus far made in the region below 5000 cm^{-1}. Since they span a considerable wavenumber range in the infra-red, they represent a convenient means of establishing the absolute accuracy of infra-red measurements, either by direct comparison in the first-order or by comparison in higher orders. The fundamental of carbon monoxide is especially suitable for this purpose because of the sharpness of its lines, convenient spacing, and freedom from underlying upper-stage bands and isotope effects. It has been used for reference purposes by Rao, Brim and Hoffman[28] on hydrogen cyanide, by Rao, Ryan and Nielsen[29] on water vapour and acetylene, and by Mould, Price and Wilkinson[30] (and other work not yet published) on ammonia, hydrogen chloride and bromide, deuterium chloride and bromide, and carbon dioxide. The wavenumbers of the lines in suitable bands of these gases have thus been compared directly with those of a band of known accuracy, and many of their values established with an accuracy approaching ±0·03 cm^{-1} or better.

On the next page the spectral ranges covered by the wavenumbers measured for the various gases are summarized, together with estimates of the absolute accuracy of the values. These measurements are of three levels of absolute accuracy: ±0·02 or better, ±0·03–0·05, and larger than ±0·05 cm^{-1}. In the first group are the bands of the diatomic molecules CO, HCl, HBr, DCl, plus two bands each of HCN and CO_2. These bands have all been measured against standard atomic lines or CO in at least two laboratories and the measurements have agreed to ±0·02 cm^{-1} or better. In the second group are those in which less confidence can be placed for any of several reasons, namely, measurement in only one laboratory at high resolution, demonstrable sensitivity of the measured values to pressure effects or to spectral slit width, and disagreement between two or more laboratories to more than ±0·02 cm^{-1}.

In the second group are combination bands of C_2H_2 and CO_2 and fundamentals of CH_4, NH_3 and N_2O. The combination bands of C_2H_2 and CO_2 have been measured in only one laboratory and those of C_2H_2 are also resolution-sensitive. The fundamentals of CH_4 and N_2O were measured in only one laboratory and are also resolution-sensitive. The widely used band of NH_3 must be assigned an accuracy no better than ±0·03 cm^{-1} at present because of the magnitude of disagreement among the three laboratories in which this band has most recently been measured at a resolution better than 0·1 cm^{-1}.

Finally, the two water bands at 3700 and 1600 cm^{-1} are in a special category. These bands would be most convenient for calibration purposes because of their ubiquity, number of peaks and broad wavenumber range. Unhappily they are very sensitive to resolution and the individual lines are easily broadened by pressure. This makes both bands very difficult to measure precisely, and also unreliable for calibration use. The band at 3700 cm^{-1} is particularly bad because of the overlapping of the two fundamentals in this region. We are therefore placing the two tables of wavenumbers for H_2O at the end of the set of tables, and are estimating the wavenumber accuracy for these bands as $\pm 0{\cdot}1$ cm^{-1}.

List of wavenumber tables, estimated precision and sources of data

Table no.	*Substance and band origin*	*Region covered by table* (cm^{-1})	*Estimated absolute accuracy* (cm^{-1})	*Sources of data*
1	CO overtone	4343–4132	±0·01	24, 25
2	C_2H_2 combination	4131–4038	±0·05	31
3	CO_2 combination	3734–3682	±0·03	32
4	CO_2 combination	3640–3579	±0·03	32
5	HCN fundamental	3386–3241	±0·01	27
6	CH_4 fundamental	3167–2936	±0·04	33
7	HCl fundamental	3060–2650	±0·02	34, 35
8	HBr fundamental	2750–2372	±0·02	34, 35
9	CO_2 fundamental	2381–2300	±0·02	33, 35
10	$^{13}CO_2$ fundamental	2295–2247	±0·02	33, 35
11	CO fundamental	2242–2013	±0·01	24, 26
12	DCl fundamental	2224–1905	±0·02	35, 36
13	DBr fundamental	1935–1727	±0·04	35, 36
14	CH_4 fundamental	1366–1248	±0·04	33
15	NH_3 fundamental	1213– 753	±0·03	30, 33, 38
16	HCN fundamental	786– 638	±0·01	27, 28
17	CO_2 fundamental	702– 629	±0·02	33, 39
18	N_2O fundamental	630– 592	±0·04	35, 36, 40
19	H_2O fundamentals*	3950–3447	±0·1	32
20	H_2O fundamental*	1890–1318	±0·1	29, 33

* The water-vapour bands are considerably inferior to the other bands listed above for calibration purposes. Unfortunately no suitable bands for the regions 4038–3734, 3579–3386, and 1727–1366 are as yet known to the Commission. This deficiency has been emphasized by placing the water-vapour bands at the end of the tables.

PROCEDURES FOR USE OF THE TABLES OF WAVENUMBERS

The two principal limitations on the accuracy with which wavenumber measurements can be made in spectrometers of moderate resolution (0·2–1 cm^{-1}) are the reproducibility of reading a specific point in a recorded spectrum (*e.g.* the position of an absorption-line maximum) and the reproducibility of the instrumental setting corresponding to a specific wavenumber. The first of these is basically set by the signal-to-noise ratio, and therefore in calibration of spectrometers the signal-to-noise ratio should be as high as possible (see p. 558). The instrumental setting is indicated in different ways by drum numbers, scale readings, pip numbers and so on, which are related to the setting of the grating or Littrow mirror. The reproducibility of the instrumental setting can be measured by repeated running of the same sharp-lined spectrum at high signal-to-noise ratio and slow scanning rate, and observing the magnitude of apparent changes in positions of the line maxima.

There are several procedures for calibrating the instrumental setting, as indicated by its scale reading, in terms of vacuum wavenumbers. These are the calibration-curve method, the interpolation method and the superposition method.

The calibration curve method

In this method the spectra of calibrating gases are obtained and the scale readings corresponding to their absorption maxima are determined. A large-scale smooth curve is then plotted with the standard vacuum wavenumbers of the maxima taken from the tables as ordinates and the scale readings of the maxima as abscissa. Wavenumbers of maxima or other desired points in unknown spectra are then determined by measurement of their scale readings and subsequent conversion to wavenumbers by reading them from the calibration curve. This procedure is rapid and simple. Its accuracy is limited by the stability of the instrument over the period of time during which the curve is assumed correct.

Interpolation method

The spectra of the calibrating gas or gases and that of the unknown are run in succession. The scale readings of the unknown are converted to vacuum wavenumbers by interpolation between the known wavenumbers of the calibrating gas. Interpolation can be linear if the spacing of the known absorption maxima is not too large or the desired accuracy is not high. The linearity can be checked by plotting a calibration curve. For non-linear interpolation, a procedure such as that proposed by McKinney and Friedel[41], Downie *et al.*[42], and Bethke[43] may be followed. For the highest precision in interpolation, interference fringes may be used[15] though these would rarely be necessary if an accuracy no higher than $\pm 0{\cdot}03$ cm^{-1} is wanted.

Superposition method

Many sources of error are eliminated or minimized by simultaneous recording of the unknown and calibration spectra. This can be done by placing two absorption cells in series. The two spectra can then be recorded as one and the interpolation procedures followed. In any event, the light path followed by the radiation should be the same for both the unknown and the calibrating gas.

Other factors which must be controlled during precise wavenumber measurement are:

Refractive index of the atmosphere in the spectrometer—The following tables give the wavenumbers in cm^{-1} *in vacuo* for the absorption maxima. If the atmosphere in the spectrometer is approximately the same as to pressure, temperature and humidity when the spectra of the unknown and the calibrating gas are recorded, the interpolated wavenumbers for the unknown will also be the values *in vacuo*. However, if the atmospheric conditions change markedly, or if the spectrum of the calibrating gas is obtained in a different grating order from that used for the unknown, appropriate correction must be made. Equations for correcting for barometric pressure and temperature are given on pp. 549 and 553 and the method for correcting for grating orders is as follows:

To compute wavenumbers *in vacuo*, ν_u vac., for an unknown (u), whose spectrum is observed in grating order M_u and in a wavenumber region where the refractive index of air is n_u, it is first necessary to correct the tabulated wavenumbers in vacuo, ν_c vac., of the calibrating gas whose spectrum is recorded in grating order M_c at the wavenumber region where the refractive index of air is n_c. The correction factor by which ν_c vac. is multiplied is $n_c M_u / n_u M_c$. If the unknown and calibration spectra are observed in the same wavenumber region, of course the refractive indices n_c and n_u are the same, and the grating orders would also be the same. The correction factor then reduces to unity.

Pressure effects on wavenumber measurement in spectra of gases—There are several pressure effects of foremost importance when high wavenumber accuracy is sought. These are pressure broadening, pressure effects on line asymmetry and pressure-induced displacement of the absorption maximum. Pressure broadening is the most important of these because the magnitude of the broadening (of the order of 0·1 to 0·3 cm^{-1} per atmosphere) approaches the spectral slit widths of spectrometers of intermediate resolution. Thus two lines observed at low pressure (say 10 mm) might have half-widths of 0·05 cm^{-1} and a readily resolvable separation of 0·5 cm^{-1}. In the presence of an inert gas at 1 atm pressure, however, the half-widths might rise to 0·3 cm^{-1} and make it quite difficult for the spectrometer to separate them. Even more important, their maxima would be drawn closer together and the apparent wavenumbers of the maxima would be in error by 0·1 cm^{-1} or perhaps more. This effort is observable for many lines in the spectrum of water vapour obtained with atmospheric moisture, and makes such lines unsuitable for calibrating use if accuracy better than $\pm 0{\cdot}1$ cm^{-1} is wanted.

When a line is asymmetric, two effects will occur if the line is observed at high pressure. The shape of the line may be changed by the pressure, which will cause a shift in the wavenumber of the maximum, and the line may be observed at too high a value of the peak absorbance, which will tend to flatten the peak and mislead the experimenter in his attempt to locate the maximum. The usual cause of line asymmetry is the superposition of several unresolved components. Such lines are poor choices for wavenumber standards, and have been avoided so far as possible in the following tables.

It can be shown on theoretical grounds, and also verified experimentally, that pressure shifts the position of a line maximum. Fortunately, at pressures of one atmosphere or less, this effect is small and need not be of concern for limits of error larger than $\pm 0{\cdot}01$ cm^{-1}.

Temperature effects—These may be divided into the effects of temperature on the spectrum and those on the instrumentation. The latter are more serious but will not be considered. Temperature can broaden lines through the Doppler effect but this is unimportant for present purposes since the broadening at room temperature for light molecules is about 0·01 cm^{-1} and is less for heavy ones. Temperature can increase vapour pressure of high-boiling liquids so that the amount of gas in an absorption cell could be strongly temperature-dependent if it is temperature-limited. The intensity of difference bands varies strongly with temperature, and if these are of appreciable intensity compared with the lines of an overlapping fundamental, the wavenumbers of the latter can be affected. This is not believed to be a serious factor in any of the bands listed in these tables and if the calibrating gases are used within 5° of the stated temperature of 25°C, no effect on wavenumber accuracy should be observable.

Electronic and mechanical effects—As was mentioned on p. 19, signal-to-noise ratio sets a basic limitation on the precision with which an absorption maximum can be located on the wavenumber scale. A spectrum on which accurate wavenumber measurements are to be made should therefore be recorded with as high a signal-to-noise ratio as can be obtained under the desired conditions of resolution and scanning time. The ratio should not be less than 30 : 1 and if possible should be much larger.

Since most spectra are now recorded automatically, the speed of recording is an important factor. Rate of recording should be slow enough so that the entire detecting, amplifying and recording system has time to reach a high fraction (say 99 per cent) of the recorded response which would be reached in an indefinitely long time. This requirement is particularly important for the sharp lines used for calibration purposes. The spectrum should also be recorded in the same direction for the calibrating gas and the unknown, and this should be the direction of smoothest wavenumber scan, as determined by the design of the driving mechanism.

TABLES OF WAVENUMBERS

The following twenty tables are illustrated by spectra obtained with a small grating spectrometer. The gaseous samples were contained in cells 10 cm long (except for *Tables 19* and *20*), at suitable pressures as indicated in the footnote to each table. These conditions refer to those under which the illustrations were obtained, and not to those used by investigators cited in the footnotes. The percentage absorption in arbitrary units is plotted upwards, and the wavenumbers in cm^{-1} are shown increasing to the left. The wavenumber scale is non-linear and is placed on the figures for convenience only. It is not intended to be an accurate scale, since the precise wavenumbers of the identified lines may be read from the adjacent table. The numbering of the lines is for identification purposes and bears no relationship to rotational quantum numbers. Occasionally, for clarity in lettering, numbers have been systematically omitted. There should be no difficulty assigning the omitted numbers to the correct lines. The chemical formula of each gas is given on its spectrum. Wavenumber values marked* in the tables are believed to be less reliable than the other values for calibration purposes because of their resolution-sensitivity, dependence on pressure or other complications.

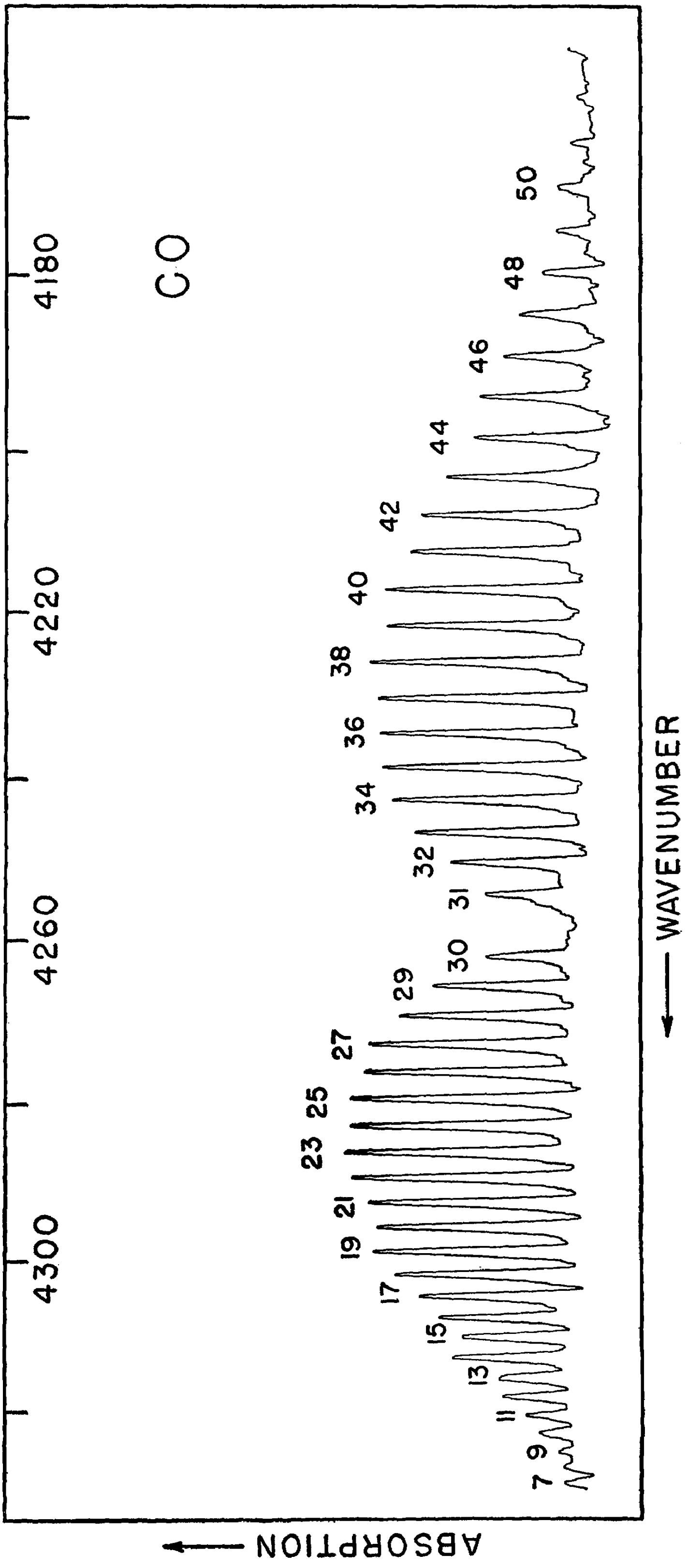
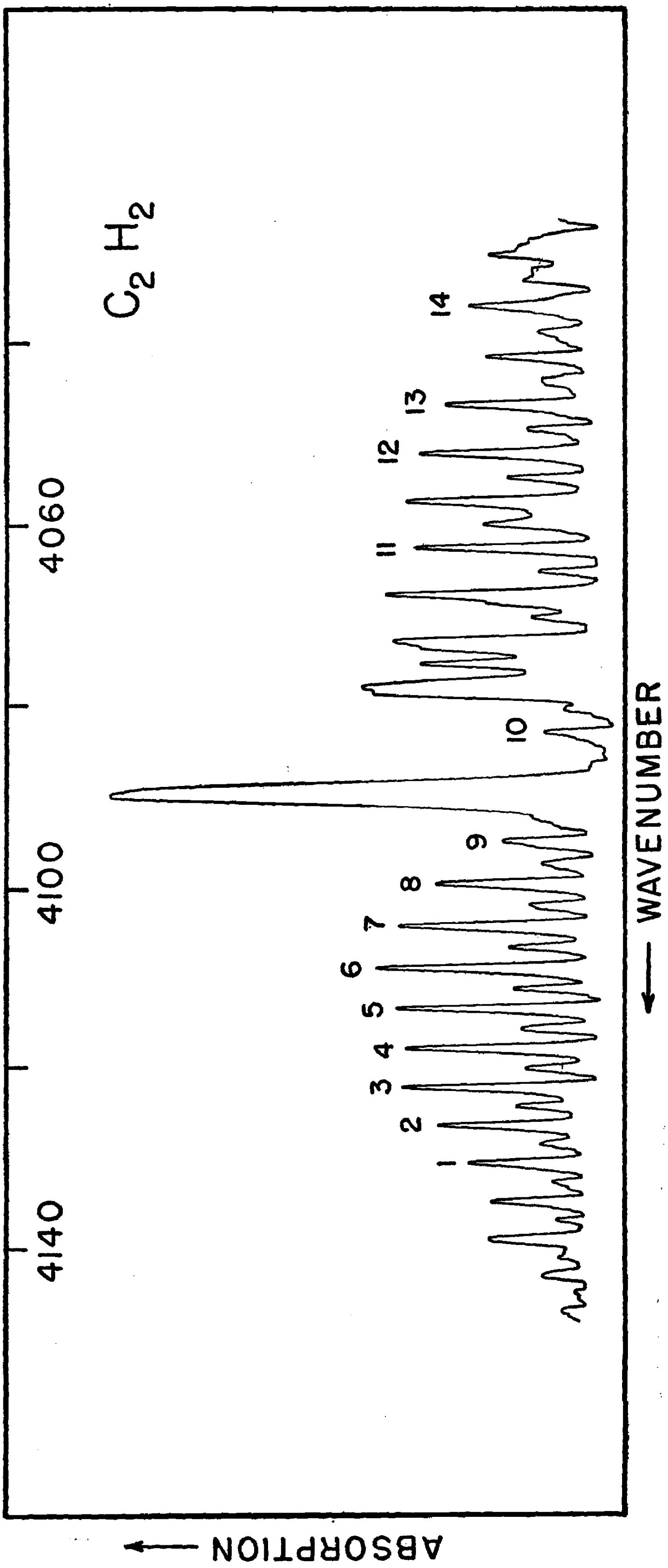

4300
4260
4220
4180
CO
7
9
11
13
15
17
19
21
23
25
27
29
30
31
32
34
36
38
40
42
44
46
48
50
← WAVENUMBER
ABSORPTION →

Table 1. Carbon monoxide overtone band: 4343–4132 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	4342·20	21	4294·64$_0$	41	4213·96$_2$
2	4340·52	22	4291·50$_6$	42	4209·35$_6$
3	4338·76	23	4288·29$_4$	43	4204·67$_3$
4	4336·93	24	4285·01$_2$	44	4199·93$_1$
5	4335·03	25	4281·65$_8$	45	4195·12$_0$
6	4333·05$_5$	26	4278·23$_5$	46	4190·23$_8$
7	4331·02	27	4274·74$_7$	47	4185·30$_0$
8	4328·88	28	4271·18$_1$	48	4180·28$_6$
9	4326·70	29	4267·54$_5$	49	4175·20$_8$
10	4324·42	30	4263·84$_0$	50	4170·06$_2$
11	4322·07$_5$	31	4256·22$_6$	51	4164·85$_2$
12	4319·65$_8$	32	4252·30$_8$	52	4159·56$_4$
13	4317·16$_7$	33	4248·33$_0$	53	4154·23$_4$
14	4314·60$_2$	34	4244·27$_3$	54	4148·81$_7$
15	4311·96$_6$	35	4240·15$_0$	55	4143·33
16	4309·26$_0$	36	4235·95$_0$	56	4137·78
17	4306·48$_2$	37	4231·69$_0$	57	4132·18
18	4303·61$_4$	38	4227·37$_1$		
19	4300·71$_2$	39	4222·96$_4$		
20	4297·70$_3$	40	4218·50$_4$		

Data from Plyler, Allen and Tidwell[25] and Rank, Guenther, Saksena, Shearer and Wiggins[24]. Cell length, 10 cm, p = 500 mm, t = 25°C, approximate spectral slit width, 1·1 cm^{-1}. The accuracy of these lines is ±0·01 cm^{-1}, and the precision somewhat better.



C2 H2
4140
4100
4060
1
2
3
4
5
6
7
8
9
10
11
12
13
14
← WAVENUMBER
← ABSORPTION

Table 2. Acetylene combination band: 4131–4038 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	4130·10	8	4100·47
2	4126·91	9	4095·84
3	4122·63	10	4084·14
4	4118·30	11	4064·58
5	4113·94	12	4054·52
6	4109·47	13	4049·36
7	4104·98*	14	4038·95

Data from Allen, Plyler and Tidwell[31]. In view of the pressure-dependence and resolution-sensitivity of this band, and of the fact that it has been measured in only one laboratory in recent years, the wavenumbers of *Table 2* are provisionally assigned a precision of ±0·03 cm^{-1}. Their accuracy is believed to be within ±0·05 cm^{-1}. Cell length, 10 cm, p = 760 mm, t = 25°C, approximate spectral slit width, 0·9 cm^{-1}.

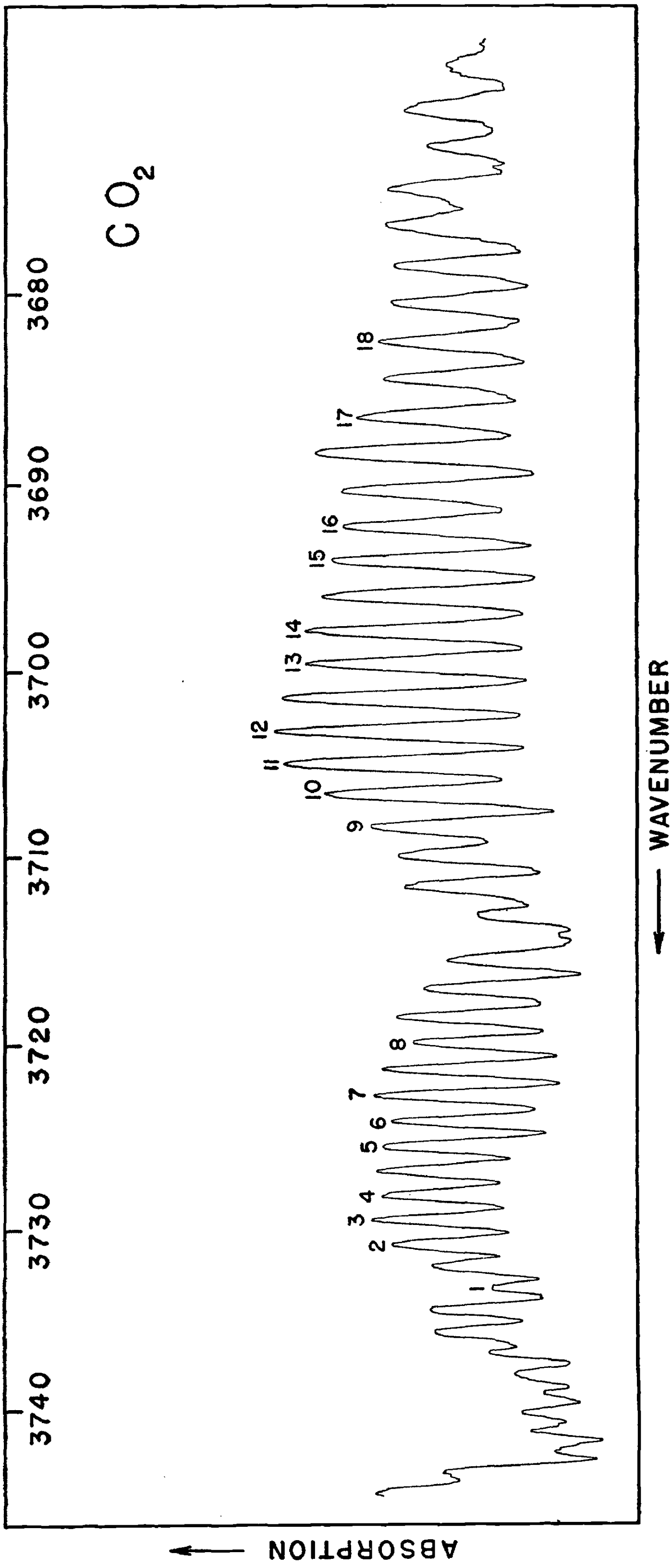

C O$_2$
3680
3690
3700
3710
3720
3730
3740
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
WAVENUMBER
ABSORPTION

Table 3. Carbon dioxide combination band: 3734–3682 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	3733·48	10	3706·70
2	3731·01	11	3705·02
3	3729·73	12	3703·29
4	3728·42	13	3699·79
5	3725·72*	14	3698·00
6	3724·35	15	3694·34*
7	3722·90	16	3692·46
8	3720·09	17	3686·74
9	3708·38	18	3682·78

Data from Plyler and Tidwell[32]. These values have been compared with those of Courtoy[44], and are regularly about 0·06 cm^{-1} higher. However, Courtoy subtracted a relatively large correction (0·1–0·2 cm^{-1}) from his measured numbers because the optical path of his interferometer beam through the spectrometer was different from that of the radiation being measured. This correction was determined by theory and apparently was not checked against a precisely known set of absorption lines. In view of this, the values of Courtoy have not been averaged with those of Plyler and Tidwell, but the latter are taken as correct within ±0·03 cm^{-1}. Cell length, 10 cm, p = 200 mm, t = 25°C, approximate spectral slit width, 0·9 cm^{-1}.

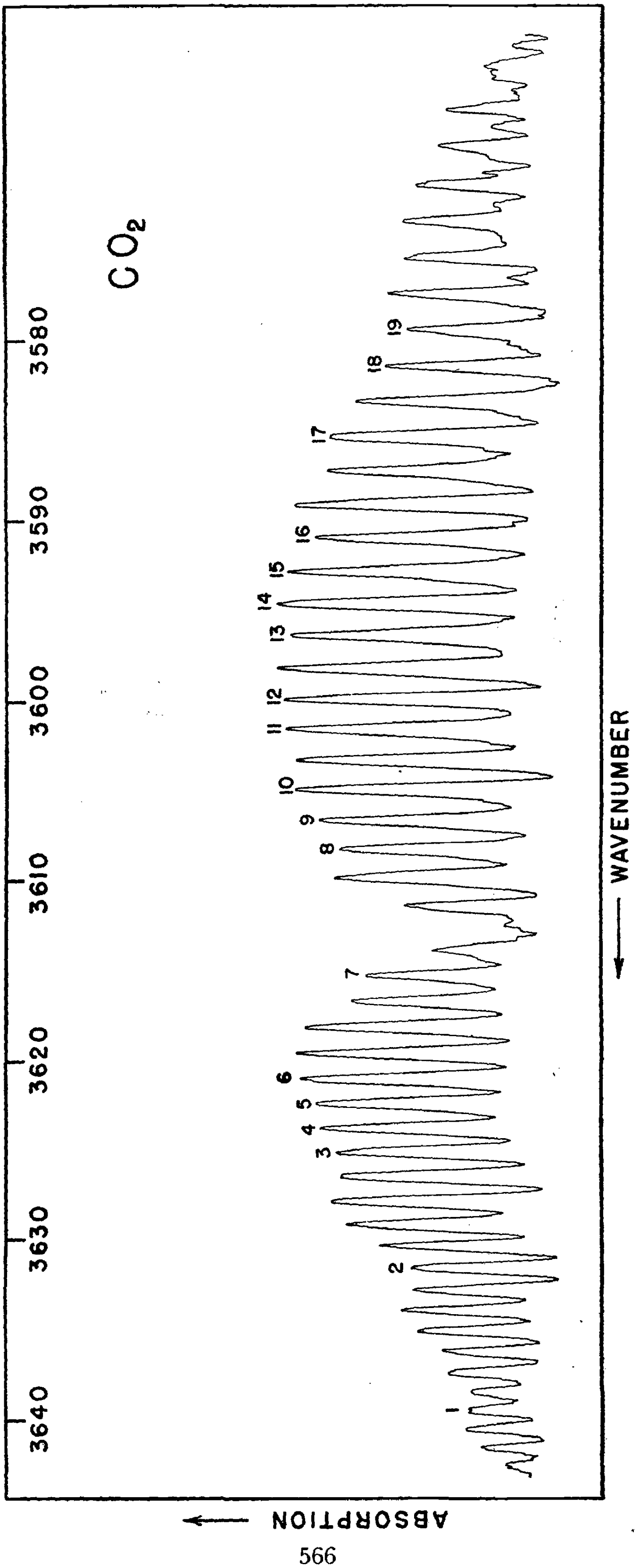

CO$_2$
3580
3590
3600
3610
3620
3630
3640
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
WAVENUMBER
ABSORPTION

Table 4. Carbon dioxide combination band: 3640–3579 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	3640·00*	11	3601·40*
2	3631·85	12	3599·74*
3	3625·27	13	3596·22
4	3623·93	14	3594·42
5	3622·50	15	3592·65*
6	3621·17*	16	3590·78
7	3615·25*	17	3585·21
8	3608·07	18	3581·31
9	3606·48	19	3579·34
10	3604·81		

Data from Plyler and Tidwell[32]. These values have been compared with those of Courtoy[44], and are regularly about 0·06 cm^{-1} higher. However, Courtoy subtracted a relatively large correction (0·1–0·2 cm^{-1}) from his measured numbers because the optical path of his interferometer beam through the spectrometer was different from that of the radiation being measured. This correction was determined by theory and apparently was not checked against a precisely known set of absorption lines. In view of this, the values of Courtoy have not been averaged with those of Plyler and Tidwell, but the latter are taken as correct within ±0·03 cm^{-1}. Cell length, 10 cm, $p = 200$ mm, $t = 25$°C, approximate spectral slit width, 0·9 cm^{-1}.

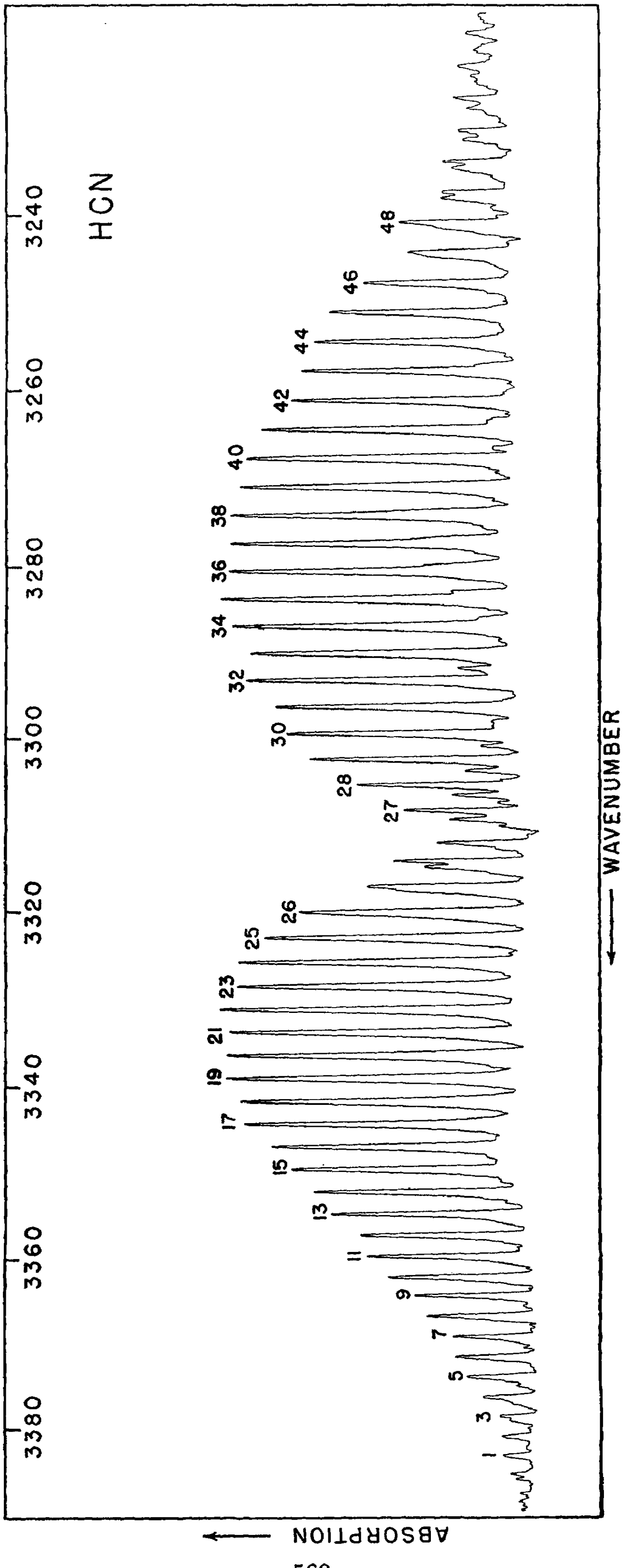
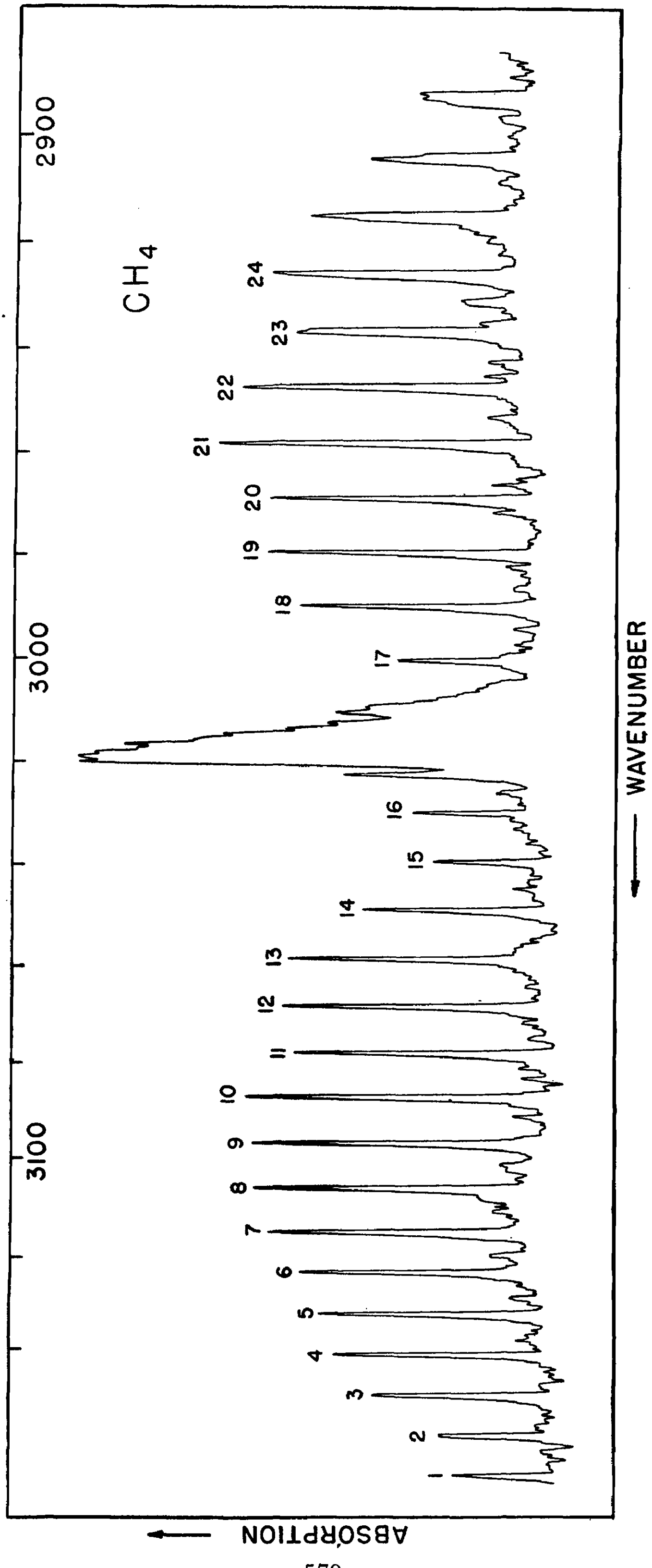

HCN
3240
3260
3280
3300
3320
3340
3360
3380
WAVENUMBER
ABSORPTION
1
3
5
7
9
11
13
15
17
19
21
23
25
26
27
28
30
32
34
36
38
40
42
44
46
48

Table 5. Hydrogen cyanide fundamental: 3386–3241 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	3385·55	17	3345·31	33	3290·34
2	3383·20	18	3342·60	34	3287·24
3	3380·83*	19	3339·88	35	3284·12
4	3378·44	20	3337·14	36	3280·98
5	3376·02	21	3334·37	37	3277·82
6	3373·59	22	3331·58	38	3274·64
7	3371·12	23	3328·77	39	3271·44
8	3368·64	24	3325·94	40	3268·22
9	3366·14	25	3323·09	41	3264·98
10	3363·61	26	3320·22	42	3261·72
11	3361·06	27	3308·52*	43	3258·44
12	3358·49	28	3305·54	44	3255·14
13	3355·90	29	3302·54	45	3251·82
14	3353·28	30	3299·52	46	3248·48
15	3350·64	31	3296·48	47	3245·12*
16	3347·99	32	3293·42	48	3241·75*

Data from Rank, Skorinko, Eastman and Wiggins[27]. These numbers are comparable in accuracy and precision to those of *Table 1.* According to these authors, the values of *Table 5,* which are smoothed values that have been checked at various lines and agree to ±0·003 cm^{-1} or better, are relatively precise to one part in 10^7 and accurate to 3 parts in 10^7. For measurements at intermediate resolution they may be relied on to ±0·01 cm^{-1}. Cell length, 10 cm, p = 20 mm, t = 25°C, approximate spectral slit width, 0·65 cm^{-1}.


CH4
2900
3000
3100
WAVENUMBER
ABSORPTION
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
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21
22
23
24

Table 6. Methane fundamental: 3167–2926 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	3166·20	13	3057·79
2	3157·61	14	3048·25
3	3148·95	15	3038·58
4	3140·20	16	3028·84
5	3131·39	17	2999·10
6	3122·46	18	2988·97*
7	3113·42	19	2979·00
8	3104·36	20	2968·67
9	3095·22	21	2958·20
10	3086·02	22	2947·92
11	3076·74	23	2937·34*
12	3067·30	24	2926·86*

Data from Plyler, Danti, Blaine and Tidwell[33]. Many of the lines of this band are resolution-sensitive, but some standard is needed to bridge the large gap between the upper lines of the hydrogen chloride fundamental and the lower frequencies of *Table 5*, which the methane fundamental does in part. Because recent high-precision work on this band has been published from only one laboratory and because of the unsatisfactory nature of many of these lines as standards, the accuracy of the values in *Table 6* is taken to be $\pm 0{\cdot}04$ cm^{-1}. Cell length, 10 cm, $p = 60$ mm, $t = 25°C$, approximate spectral slit width, 0·65 cm^{-1}.

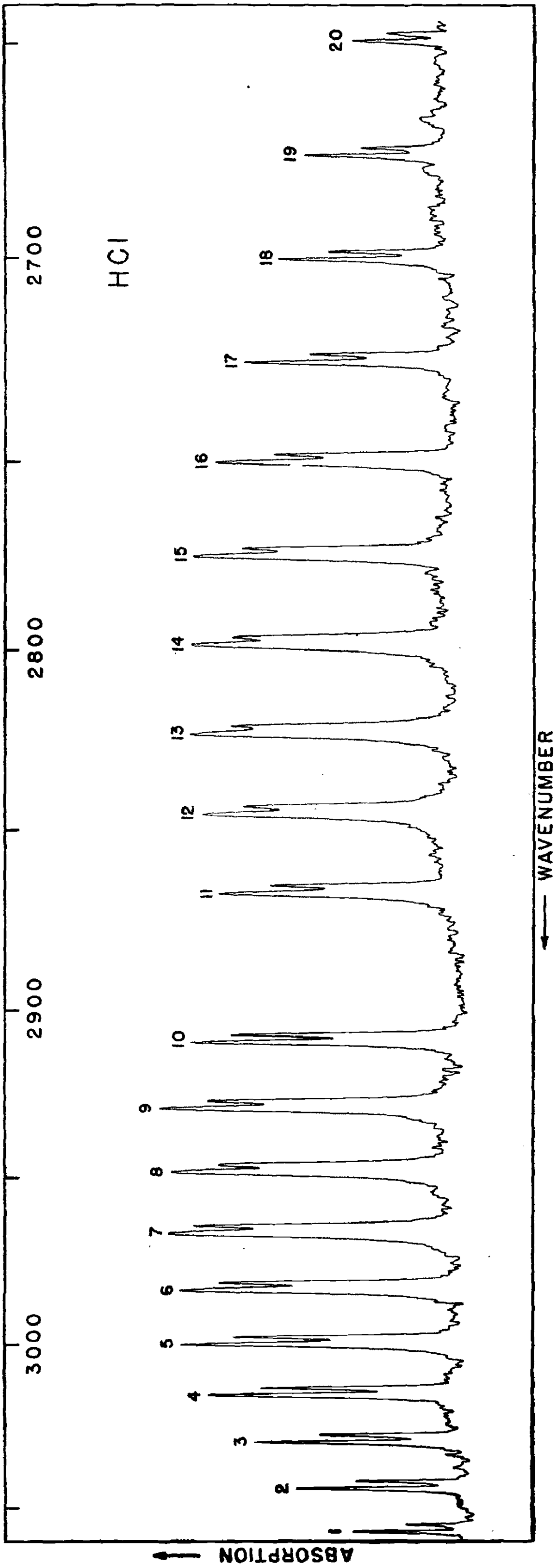

HCl
3000
2900
2800
2700
WAVENUMBER
ABSORPTION
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

Table 7. Hydrogen chloride fundamental: 3060–2650 cm^{-1}

Line pair no.	*Wavenumber* (vac.) (cm^{-1})		*Line pair no.*	*Wavenumber* (vac.) (cm^{-1})	
	$H^{35}Cl$	$H^{37}Cl$		$H^{35}Cl$	$H^{37}Cl$
1	3059·32	3056·97	11	2865·10	2863·02
2	3045·06	3042·73	12	2843·62	2841·58
3	3030·09	3027·78	13	2821·56	2819·56
4	3014·41	3012·12	14	2798·94	2796·97
5	2998·04	2995·78	15	2775·76	2773·82
6	2981·00	2978·75	16	2752·04	2750·13
7	2963·29	2961·07	17	2727·78	2725·92
8	2944·90	2942·72	18	2703·01	2701·18
9	2925·90	2923·72	19	2677·73	2675·94
10	2906·24	2904·11	20	2651·96	2650·22

Data are from Plyler and Tidwell[34] and Mould, Price and Wilkinson[35]. The agreement of these two laboratories is very close. The relative precision is ±0·01 cm^{-1} and the accuracy ±0·02 cm^{-1}. Cell length, 10 cm, $p = 250$ mm, $t = 25°C$, approximate spectral slit width, 0·7 cm^{-1}.

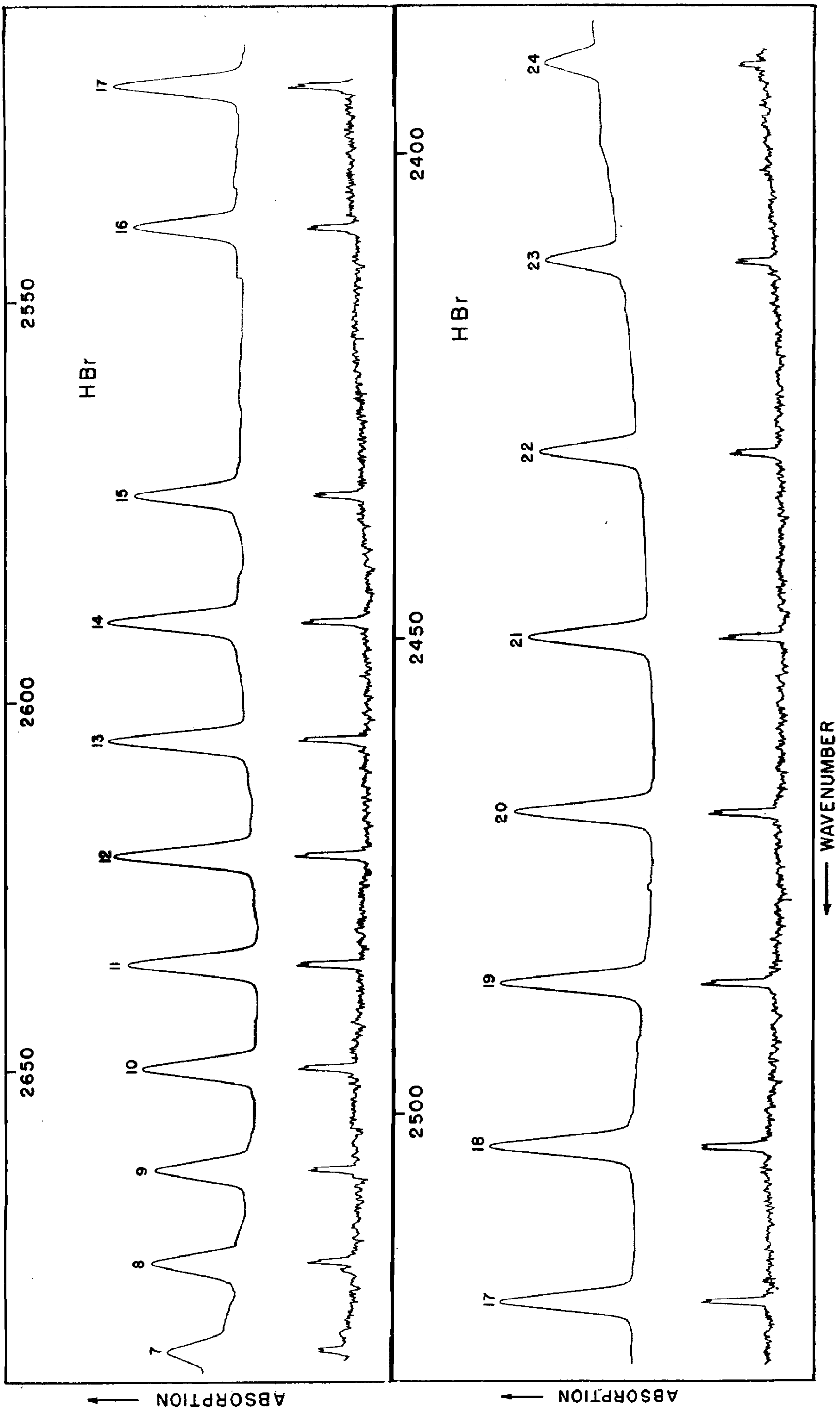
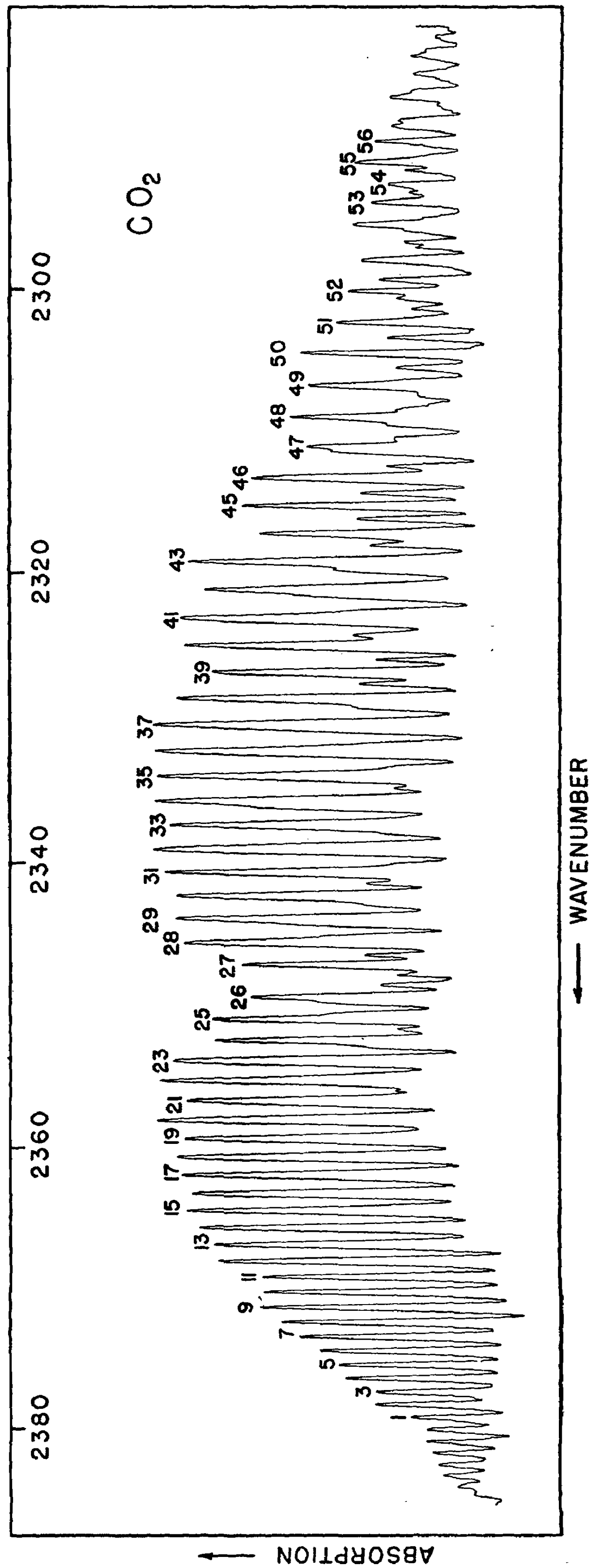

2650
2600
2550
HBr
7
8
9
10
11
12
13
14
15
16
17
2500
2450
2400
HBr
17
18
19
20
21
22
23
24
ABSORPTION
ABSORPTION
WAVENUMBER

Table 8. Hydrogen bromide fundamental: 2750–2372 cm^{-1}

Line pair no.	*Wavenumber* (vac.) (cm^{-1}) $H^{79}Br$	$H^{81}Br$	*av.*	*Line pair no.*	*Wavenumber* (vac.) (cm^{-1}) $H^{79}Br$	$H^{81}Br$	*av.*
1	2749·33	2748·90	2749·12	16	2542·25	2541·87	2542·06
2	2740·42	2739·98	2740·20	17	2525·09	2524·72	2524·91
3	2730·93	2730·49	2730·71	18	2507·48	2507·12	2507·30
4	2720·87	2720·44	2720·66	19	2489·43	2489·08	2489·26
5	2710·26	2709·84	2710·05	20	2470·96	2470·61	2470·79
6	2699·10	2698·68	2698·89	21	2452·07	2451·72	2451·90
7	2687·40	2686·97	2687·19	22	2432·76	2432·42	2432·59
8	2675·16	2674·74	2674·95	23	2413·06	2412·72	2412·89
9	2662·40	2661·98	2662·19	24	2392·96	2392·63	2392·80
10	2649·12	2648·71	2648·92	25	2372·45	2372·13	2372·29
11	2635·32	2634·92	2635·12				
12	2621·02	2620·62	2620·82				
13	2606·23	2605·83	2606·03				
14	2590·95	2590·56	2590·76				
15	2575·19	2574·80	2575·00				

Data are from Plyler and Tidwell[36] and Mould, Price and Wilkinson[35]. The agreement between the two sets of data is very close. The relative precision is ±0·01 cm^{-1} and the accuracy ±0·02 cm^{-1}. A study by Plyler, Danti, Blaine and Tidwell[33] shows that for spectrometers of insufficient resolving power to separate the $H^{79}Br—H^{81}Br$ doublet cleanly, the measured centre of gravity of the doublet is given within the accuracy of the measurement by the average of the high-resolution values for the components. This average is therefore included in *Table 8.* Cell length, 10 cm, p = 60 and 140 mm, t = 25°C, approximate spectral slit width, 0·5 and 0·8 cm^{-1}.


CO_2
2300
2320
2340
2360
2380
WAVENUMBER
ABSORPTION
1
3
5
7
9
11
13
15
17
19
21
23
25
26
27
28
29
31
33
35
37
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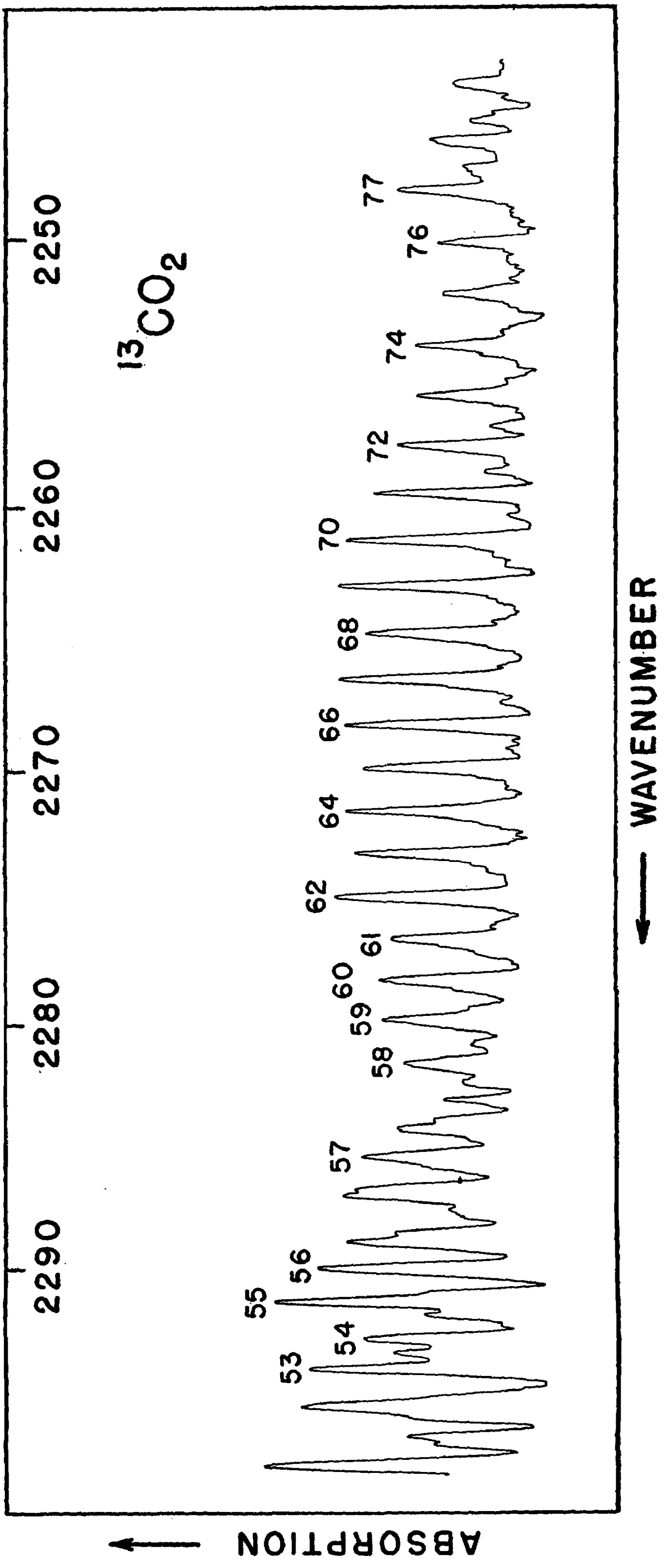
56

Table 9. Carbon dioxide fundamental: 2381–2300 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	2380·74	21	2357·37	41	2323·10
2	2379·80	22	2355·94	42	2321·16
3	2378·86	23	2354·48	43	2319·20
4	2377·88	24	2353·00*	44	2317·22
5	2376·87	25	2351·50*	45	2315·21
6	2375·83	26	2349·96*	46	2313·18
7	2374·79	27	2347·62*	47	2311·12
8	2372·70	28	2346·03*	48	2309·05
9	2373·61	29	2344·41*	49	2306·95
10	2371·47	30	2342·77	50	2304·84
11	2370·32	31	2341·11	51	2302·69
12	2369·12	32	2339·42	52	2300·50*
13	2367·92	33	2337·70		
14	2366·69	34	2335·96*	53	2294·45*
15	2365·41	35	2334·19	54	2293·10*
16	2364·15	36	2332·40	55	2291·62*
17	2362·85	37	2330·59	56	2290·23
18	2361·51	38	2328·76*		(Lines 53–56 from carbon-13 dioxide)
19	2360·16	39	2326·90		
20	2358·77	40	2325·01		

Data from Plyler, Danti, Blaine and Tidwell[33] and Mould, Price and Wilkinson[35]. The measurements agree to better than ±0·02. The values of Mould, Price and Wilkinson were smoothed values. It is estimated that the precision is ±0·01 cm^{-1} and the absolute accuracy is ±0·02 cm^{-1} except for the starred lines. Cell length, 10 cm, p = 30 mm, t = 25°C, approximate spectral slit width, 0·5 cm^{-1}.


2250
2260
2270
2280
2290
13CO2
53
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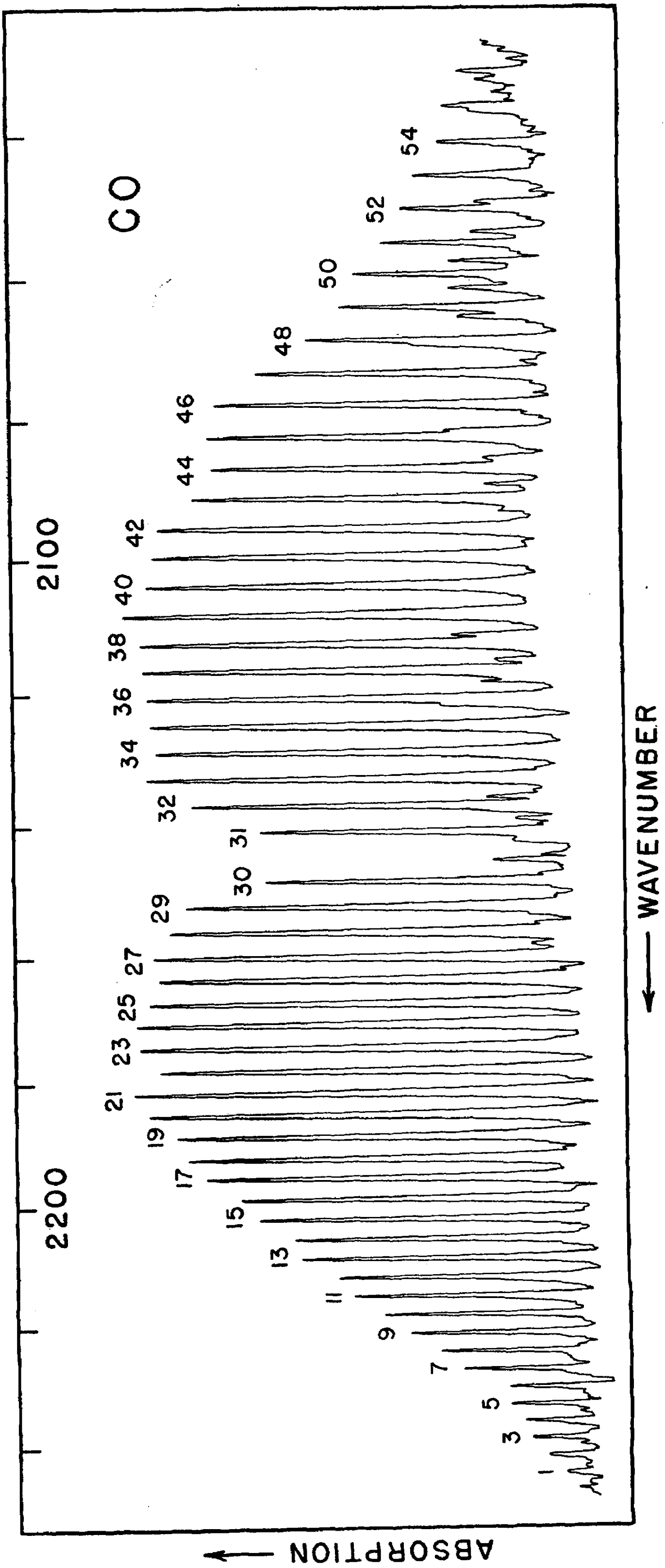
74
76
77
WAVENUMBER
ABSORPTION

Table 10. Carbon-13 dioxide fundamental: 2295–2247 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
53	2294·45*	66	2268·55
54	2293·10*	67	2266·76
55	2291·62*	68	2264·96
56	2290·23	69	2263·14
57	2285·79*	70	2261·29
58	2281·93*	71	2259·42
59	2280·33	72	2257·52
60	2278·71	73	2255·60
61	2277·09	74	2253·66
62	2275·42	75	2251·69
63	2273·74	76	2249·68
64	2272·03	77	2247·68
65	2270·30		

Data from Plyler, Danti, Blaine and Tidwell[33] and Mould, Price and Wilkinson[35]. The measurements agree to better than ±0·02. The values of Mould, Price and Wilkinson were smoothed values. It is estimated that the precision is ±0·01 cm^{-1} and the absolute accuracy is ±0·02 cm^{-1} except for the starred lines. Cell length, 10 cm, p = 50 mm, t = 25°C, approximate spectral slit width, 0·5 cm^{-1}.


CO
2100
2200
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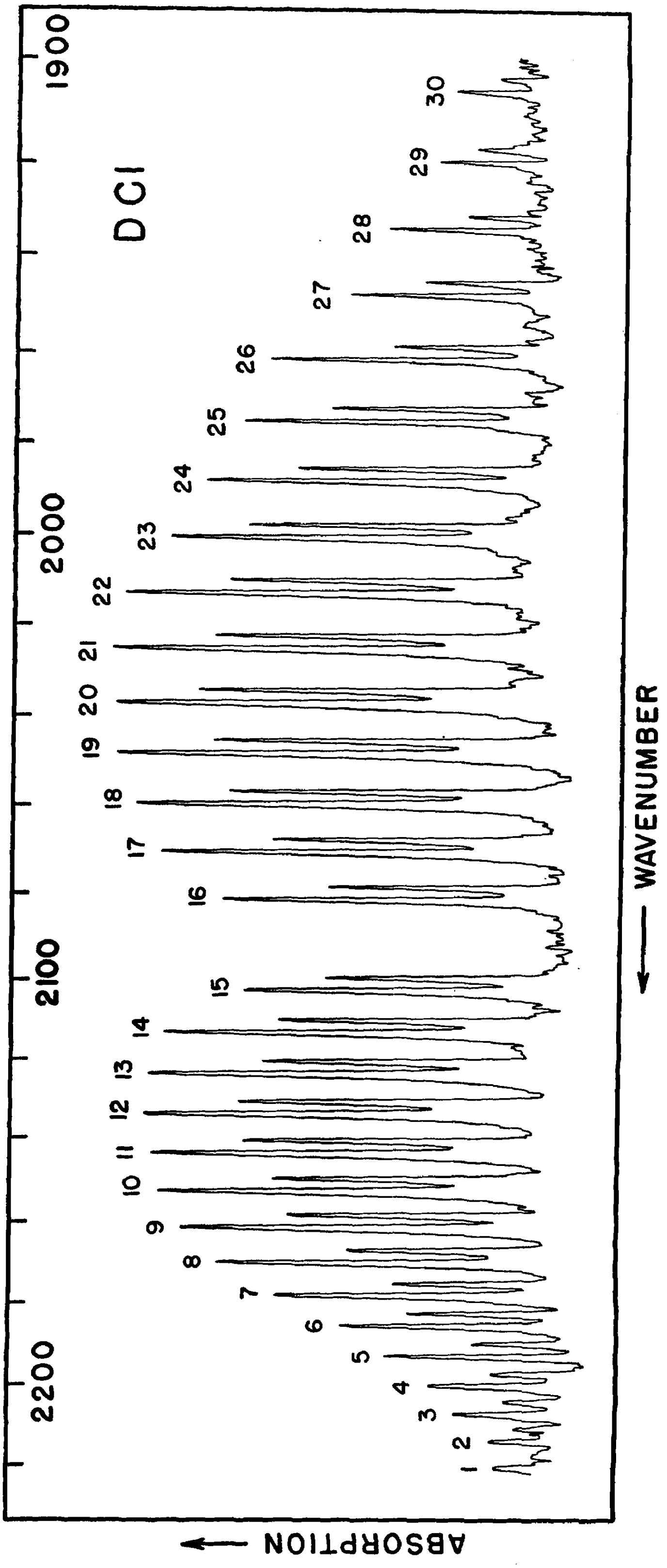
WAVENUMBER
ABSORPTION

Table 11. Carbon monoxide fundamental: 2242–2013 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	$2241{\cdot}68_{5}$	21	$2179{\cdot}77_{0}$	41	$2099{\cdot}09_{0}$
2	$2238{\cdot}95_{8}$	22	$2176{\cdot}28_{6}$	42	$2094{\cdot}86_{6}$
3	$2236{\cdot}18_{6}$	23	$2172{\cdot}76_{0}$	43	$2090{\cdot}61_{0}$
4	$2233{\cdot}36_{2}$	24	$2169{\cdot}20_{0}$	44	$2086{\cdot}32_{3}$
5	$2230{\cdot}52_{6}$	25	$2165{\cdot}60_{4}$	45	$2082{\cdot}00_{6}$
6	$2227{\cdot}63_{8}$	26	$2161{\cdot}97_{1}$	46	$2077{\cdot}65_{1}$
7	$2224{\cdot}71_{2}$	27	$2158{\cdot}30_{5}$	47	$2073{\cdot}26_{5}$
8	$2221{\cdot}75_{0}$	28	$2154{\cdot}59_{8}$	48	$2068{\cdot}85_{0}$
9	$2218{\cdot}74_{6}$	29	$2150{\cdot}86_{0}$	49	$2064{\cdot}39_{7}$
10	$2215{\cdot}70_{5}$	30	$2147{\cdot}08_{5}$	50	$2059{\cdot}91_{4}$
11	$2212{\cdot}62_{4}$	31	$2139{\cdot}43_{0}$	51	$2055{\cdot}40_{0}$
12	$2209{\cdot}51_{0}$	32	$2135{\cdot}55_{0}$	52	$2050{\cdot}85_{5}$
13	$2206{\cdot}35_{4}$	33	$2131{\cdot}63_{5}$	53	$2046{\cdot}27_{6}$
14	$2203{\cdot}16_{0}$	34	$2127{\cdot}68_{6}$	54	$2041{\cdot}66_{5}$
15	$2199{\cdot}93_{3}$	35	$2123{\cdot}70_{2}$	55	$2037{\cdot}03_{0}$
16	$2196{\cdot}66_{4}$	36	$2119{\cdot}68_{4}$	56	$2032{\cdot}35_{3}$
17	$2193{\cdot}36_{0}$	37	$2115{\cdot}63_{2}$	57	$2027{\cdot}65_{0}$
18	$2190{\cdot}02_{0}$	38	$2111{\cdot}55_{0}$	58	$2022{\cdot}91_{0}$
19	$2186{\cdot}64_{0}$	39	$2107{\cdot}42_{5}$	59	$2018{\cdot}15$
20	$2183{\cdot}22_{6}$	40	$2103{\cdot}27_{0}$	60	$2013{\cdot}35$

Data are from Plyler, Blaine and Connor[26], and the calculations of Rank and co-workers[24]. These two sets of values agree so closely that small errors due to optical displacement of standard and sample, lack of coincidences between orders, and uncertainty in the refractive index of air appear to have been reduced well below 0·01 cm^{-1}. Because of the sharpness and convenient spacing of the lines and freedom from underlying bands, this band is an excellent reference standard for assessment of the absolute accuracy of infra-red wavenumbers measured in absorption in gases. The values listed are considered reliable to $\pm 0{\cdot}01$ cm^{-1} in absolute accuracy. Cell length, 10 cm, $p = 150$ mm, $t = 25$°C, approximate spectral slit width, 0·45 cm^{-1}.



DCl
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2200
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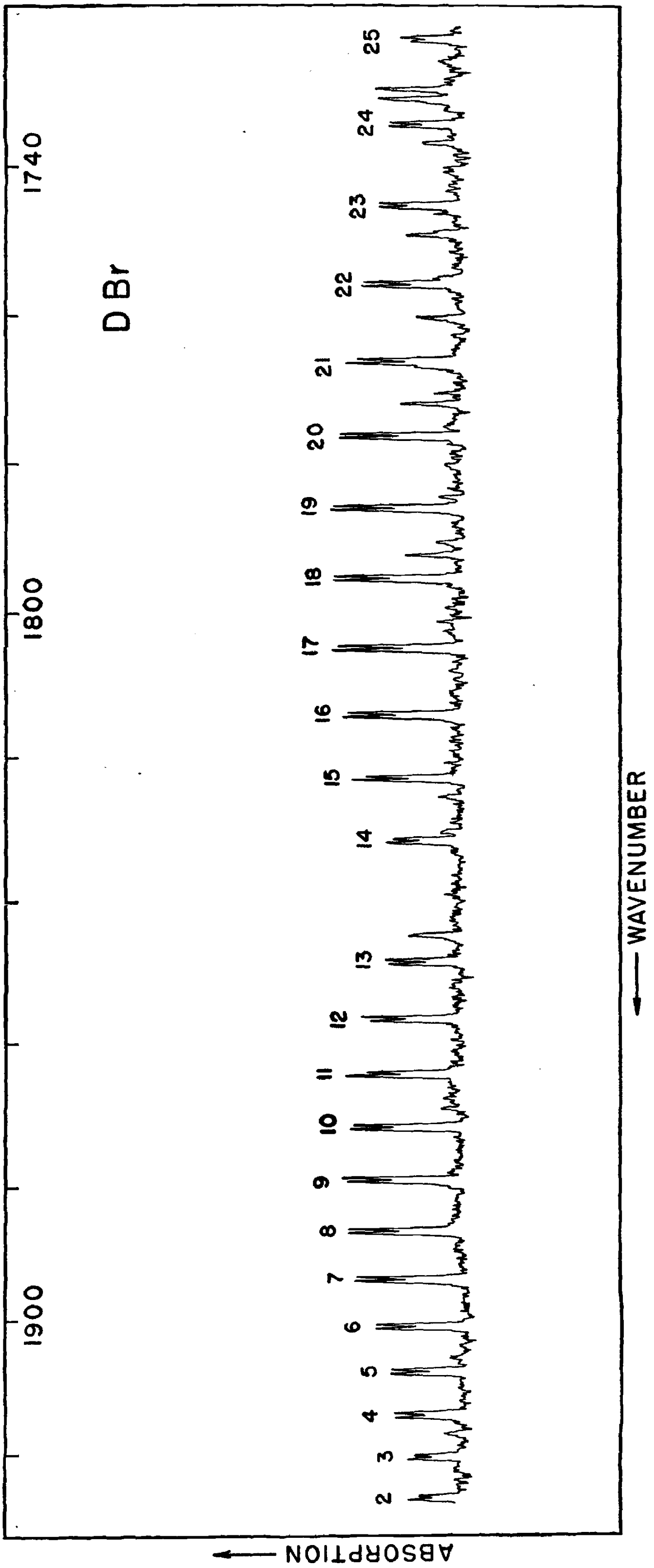
WAVENUMBER
ABSORPTION

Table 12. Deuterium chloride fundamental: 2224–1905 cm^{-1}

Line pair no.	*Wavenumber* (vac.) (cm^{-1}) $D^{35}Cl$	*Wavenumber* (vac.) (cm^{-1}) $D^{37}Cl$	*Line pair no.*	*Wavenumber* (vac.) (cm^{-1}) $D^{35}Cl$	*Wavenumber* (vac.) (cm^{-1}) $D^{37}Cl$
1	2224·04	2220·70	16	2080·28	2077·31
2	2216·96	2213·64	17	2069·27	2066·34
3	2209·62	2206·31	18	2058·05	2055·15
4	2202·00	2198·71	19	2046·61	2043·75
5	2194·13	2190·86	20	2034·96	2032·13
6	2186·00	2182·74	21	2023·10	2020·31
7	2177·61	2174·37	22	2011·04	2008·28
8	2168·96	2165·75	23	1998·78	1996·06
9	2160·07	2156·88	24	1986·32	1983·64
10	2150·93	2147·76	25	1973·66	1971·02
11	2141·54	2138·40	26	1960·82	1958·22
12	2131·91	2128·80	27	1947·78	1945·22
13	2122·05	2118·96	28	1934·57	1932·05
14	2111·95	2108·89	29	1921·17	1918·69
15	2101·62	2098·59	30	1907·59	1905·16

Data from Mould, Price and Wilkinson[35] and Plyler[36]. Cell length, 10 cm, p = 250 mm, t = 25°C, approximate spectral slit width, 0·6–1·0 cm^{-1}.


DBr
1740
1800
1900
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
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24
25
WAVENUMBER
ABSORPTION

Table 13. Deuterium bromide fundamental: 1935–1727 cm^{-1}

Line pair no.	*Wavenumber* (vac.) (cm^{-1}) $D^{79}Br$	$D^{81}Br$	*av.*	*Line pair no.*	*Wavenumber* (vac.) (cm^{-1}) $D^{79}Br$	$D^{81}Br$	*av.*
1	1934·54	1933·93	1934·23	14	1831·59	1831·05	1831·32
2	1928·38	1927·79	1928·09	15	1822·93	1822·40	1822·67
3	1922·04	1921·44	1921·74	16	1814·10	1813·57	1813·83
4	1915·49	1914·90	1915·20	17	1805·12	1804·60	1804·86
5	1908·77	1908·17	1908·47	18	1795·97	1795·46	1795·72
6	1901·86	1901·27	1901·57	19	1786·67	1786·16	1786·42
7	1894·76	1894·17	1894·47	20	1777·22	1776·72	1776·97
8	1887·48	1886·90	1887·19	21	1767·61	1767·11	1767·36
9	1880·02	1879·45	1879·74	22	1757·86	1757·37	1757·62
10	1872·38	1871·81	1872·10	23	1747·96	1747·47	1747·72
11	1864·57	1864·01	1864·29	24	1737·92	1737·43	1737·68
12	1856·58	1856·02	1856·30	25	1727·74	1727·25	1727·50
13	1848·42	1847·87	1848·15				

Data from Mould, Price and Wilkinson[35] and Plyler[36]. Cell length, 10 cm, $p = 60$ mm, $t = 25$°C, approximate spectral slit width, 0·5–0·65 cm^{-1}.

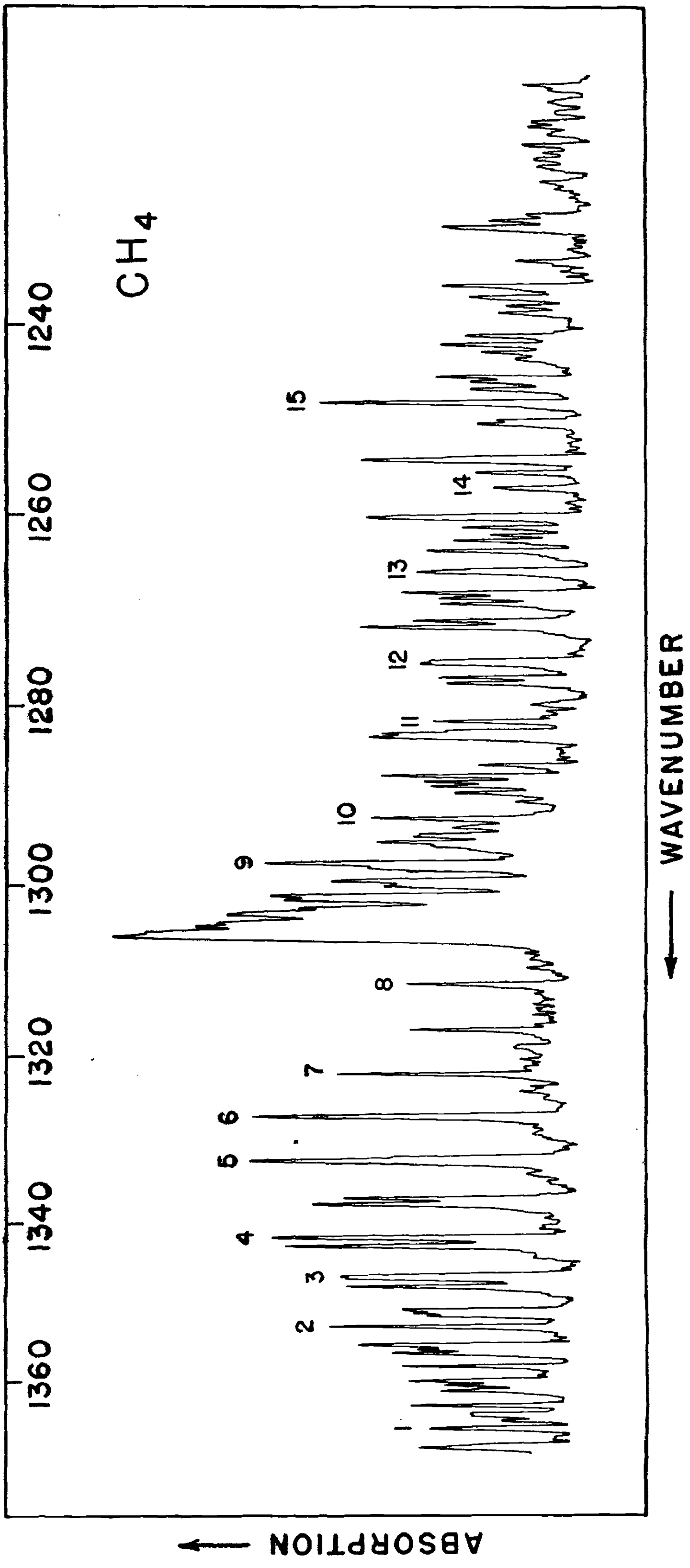

CH$_4$
1360
1340
1320
1300
1280
1260
1240
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
← WAVENUMBER
← ABSORPTION

Table 14. Methane fundamental: 1366–1248 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	1366·04	9	1297·63*
2	1353·06	10	1292·61
3	1346·70*	11	1281·59
4	1341·79*	12	1275·20*
5	1332·41*	13	1265·52*
6	1327·20	14	1256·60
7	1322·09	15	1247·81
8	1311·42*		

Data from Plyler, Danti, Blaine and Tidwell[33] only. No measurements of comparable precision are available for comparison. These lines are resolution-sensitive, particularly those starred. Except for the latter, an absolute accuracy of ±0·03 is provisionally assigned. For values more suited to calibration of spectrometers with spectral slit widths of 1 cm^{-1} or larger, see Part II of these tables. Cell length, 10 cm, p = 60 mm, t = 25°C, approximate spectral slit width, 0·34 cm^{-1}.

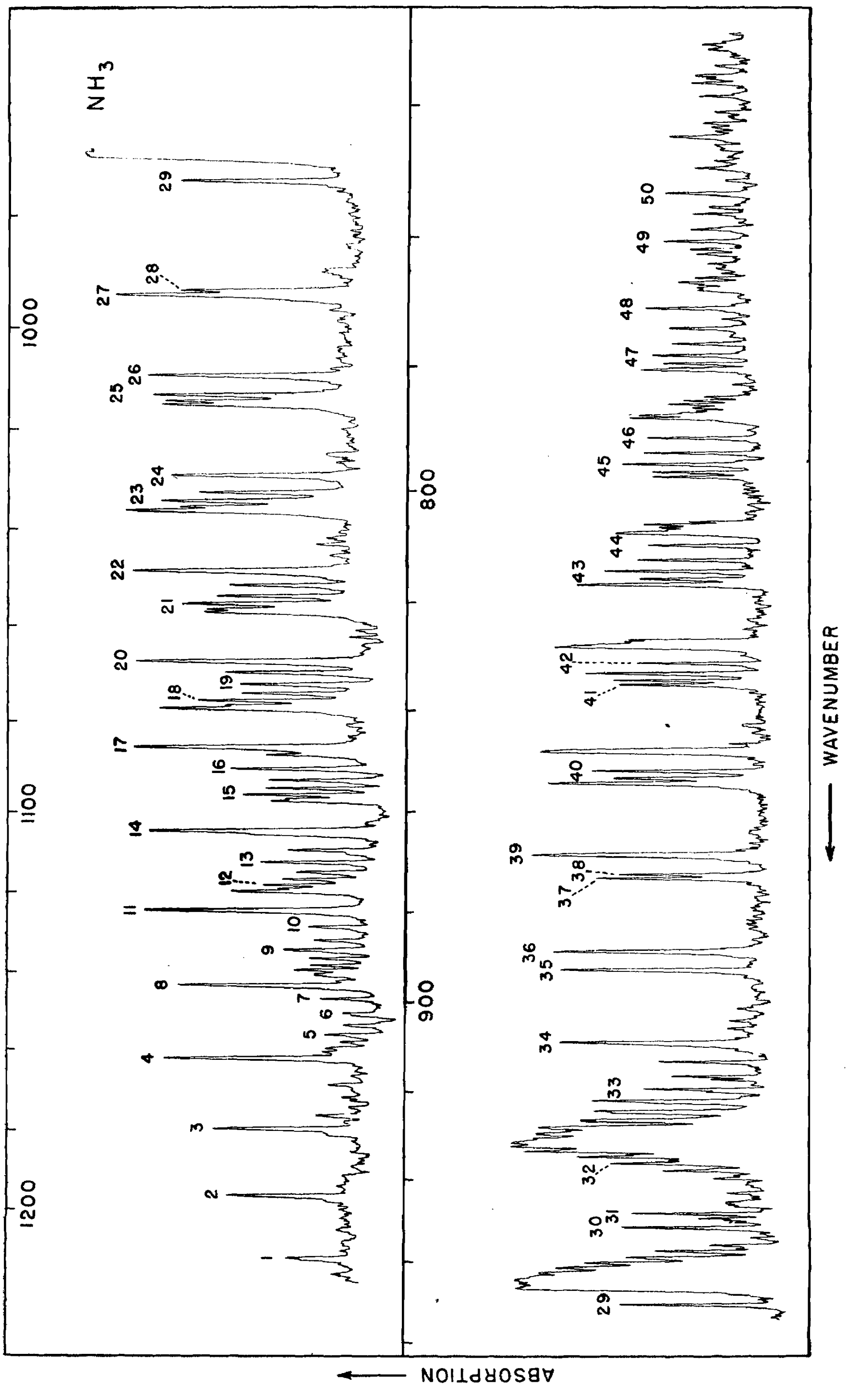
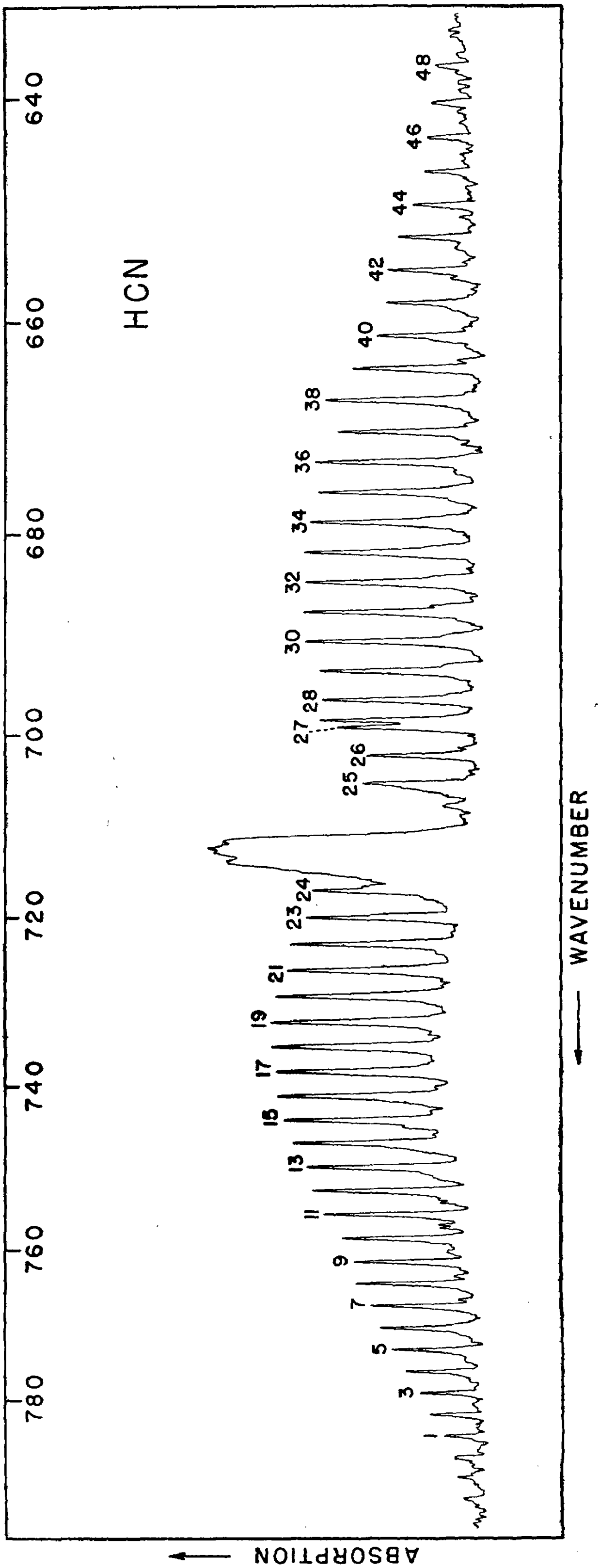

NH$_3$
1200
1100
1000
900
800
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50
ABSORPTION
WAVENUMBER

Table 15. Ammonia fundamental: 1213–753 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	1212·68*	19	1070·59	37	872·58
2	1195·00	20	1065·57	38	871·74
3	1177·09	21	1053·14	39	867·81*
4	1158·95	22	1046·41	40	851·35
5	1152·86*	23	1032·13	41	834·84
6	1147·53*	24	1027·04	42	830·68
7	1143·90	25	1011·21	43	814·24
8	1140·64	26	1007·55	44	809·72
9	1131·86	27	992·60*	45	796·15
10	1126·03	28	991·70*	46	791·74
11	1122·14	29	971·91	47	778·29
12	1116·03	30	951·80	48	770·92
13	1110·68	31	948·25	49	760·70
14	1103·44	32	935·90	50	753·61
15	1095·15*	33	918·62		
16	1089·39	34	908·18		
17	1084·61	35	892·04*		
18	1074·16	36	888·00		

Data from Plyler, Danti, Blaine and Tidwell[33], Mould, Price and Wilkinson[30] and Garing[39]. Agreement among these three independent sets of data indicates that the absolute accuracy of most of the lines is about ±0·03 cm^{-1} except for the starred lines, which are resolution-sensitive. Mould, Price and Wilkinson give wavenumbers for many additional lines suitable for calibration. Cell length, 10 cm, p = 50 mm, t = 25°C, approximate spectral slit width, 0·5 cm^{-1}.


HCN
ABSORPTION
WAVENUMBER
640
660
680
700
720
740
760
780
1
3
5
7
9
11
13
15
17
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21
23
24
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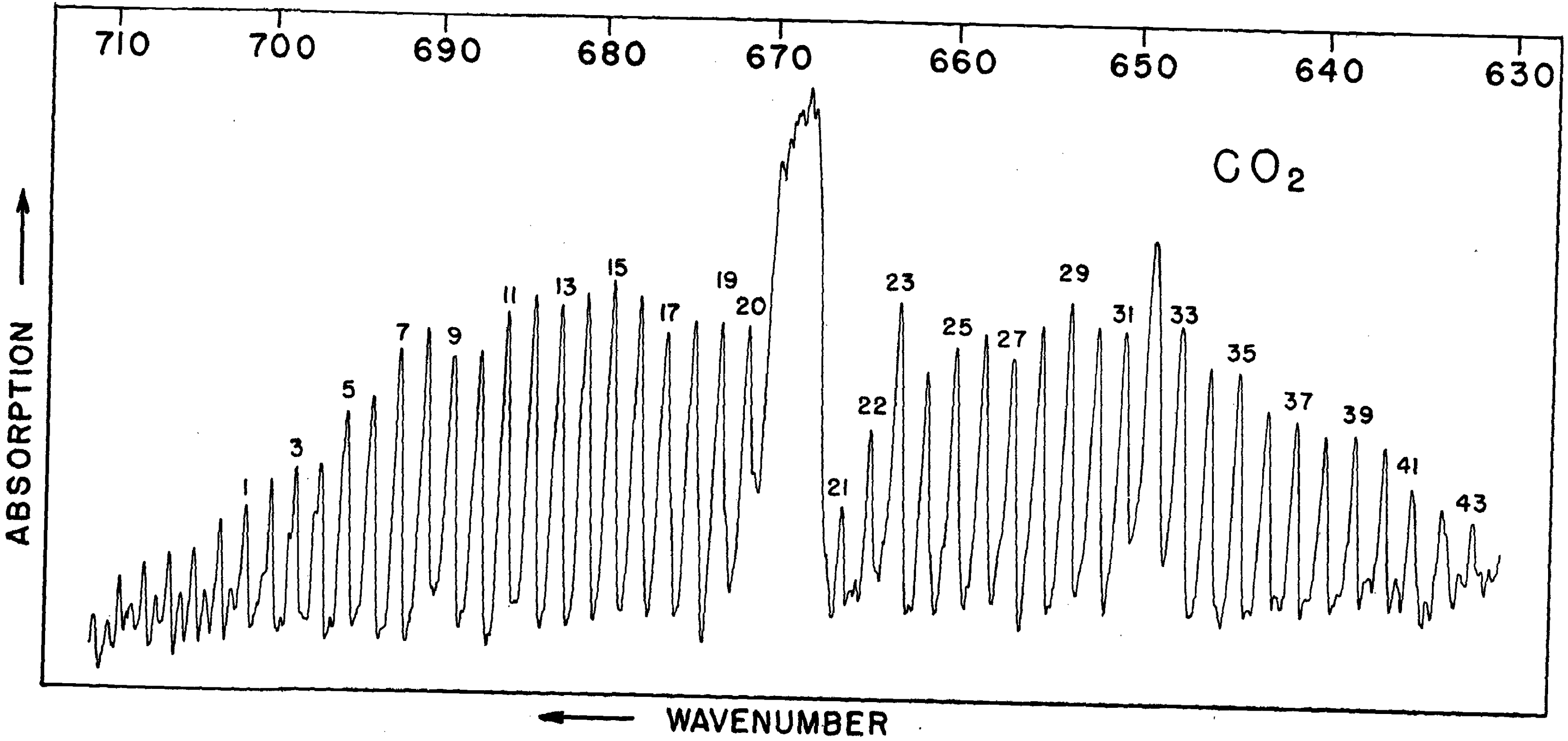
46
48

Table 16. Hydrogen cyanide fundamental: 786–638 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	785·57	17	738·57	33	682·40
2	782·65	18	735·61	34	679·45
3	779·72	19	732·66	35	676·49
4	776·79	20	729·72	36	673·54
5	773·87	21	726·76	37	670·60
6	770·94	22	723·80	38	667·64
7	768·00	23	720·85	39	664·68
8	765·06	24	717·90*	40	661·73
9	762·14	25	706·08*	41	658·77
10	759·19	26	703·12	42	655·82
11	756·26	27	700·16*	43	652·88
12	753·31	28	697·19	44	649·91
13	750·37	29	694·24	45	646·97
14	747·40	30	691·29	46	644·03
15	744·45	31	688·34	47	641·07
16	741·51	32	685·36	48	638·13

Data from Rao, Brim and Hoffman[28]. The measured values of Rao, Brim and Hoffman check those calculated by Rank *et al.*[27] with the help of the combination principle to better than 0·01 cm^{-1} for most lines of low J-value. Hence the absolute accuracy of most of the numbers in *Table 16* is ±0·01 cm^{-1}. Cell length, 10 cm, $p = 30$ mm, $t = 25°C$, approximate spectral slit width, 0·4 cm^{-1}.


710
700
690
680
670
660
650
640
630
CO$_2$
ABSORPTION
1
3
5
7
9
11
13
15
17
19
20
21
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27
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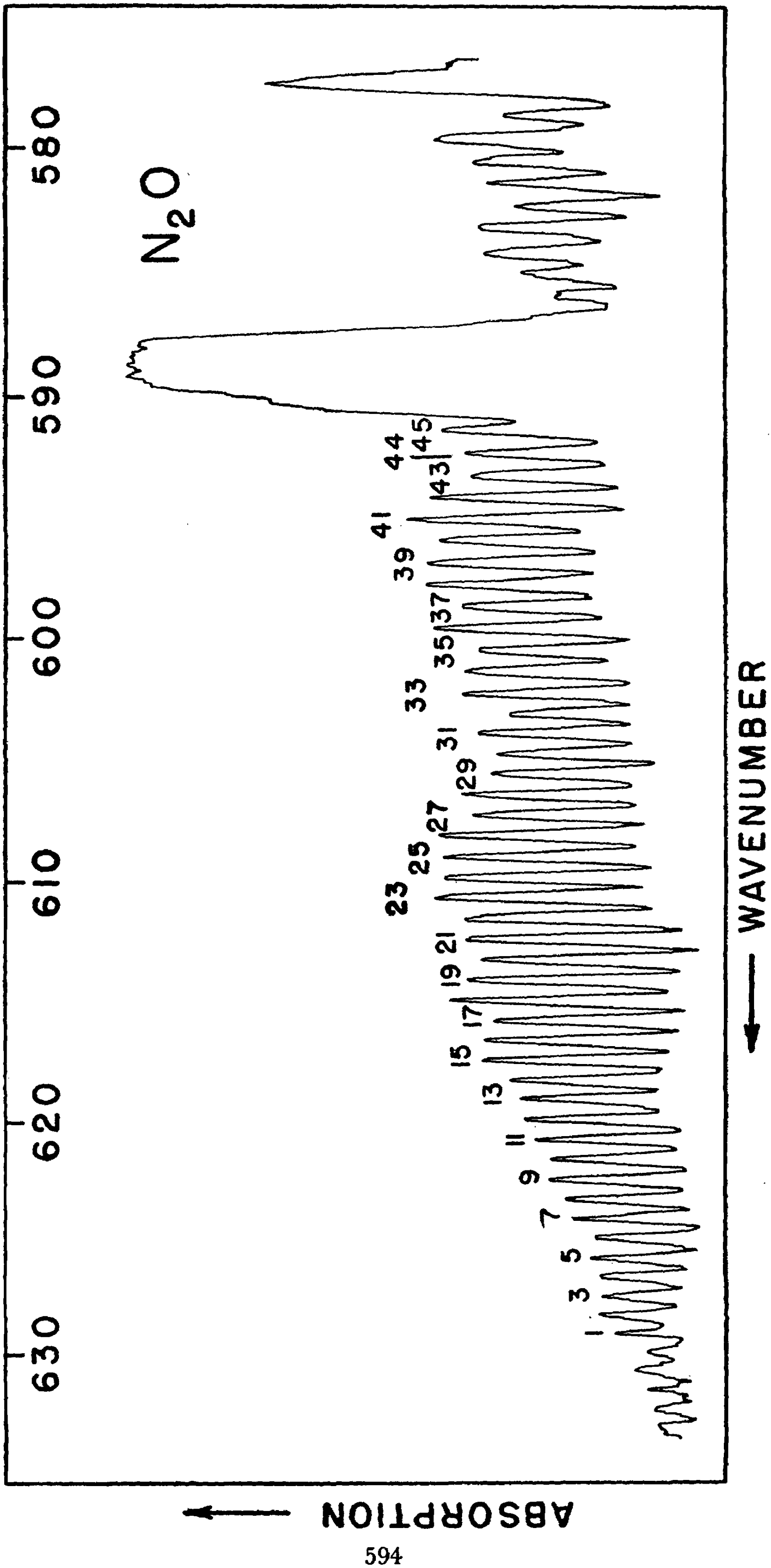
33
35
37
39
41
43
WAVENUMBER

Table 17. Carbon dioxide fundamental: 702–629 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	701·69	16	677·60	31	650·40
2	700·07	17	676·04	32	648·90
3	698·44	18	674·45	33	647·39
4	696·82	19	672·88	34	645·90
5	695·19	20	671·34	35	644·37
6	693·59	21	665·83	36	642·86
7	691·98	22	664·28	37	641·37
8	690·37	23	662·71	38	639·83
9	688·78	24	661·17	39	638·34
10	687·16	25	659·60*	40	636·87
11	685·55	26	658·07	41	635·38
12	683·96	27	656·53	42	633·88
13	682·37	28	655·00	43	632·42
14	680·78	29	653·48	44	630·93
15	679·20	30	651·94	45	629·46

Data from Rossmann, Rao and Nielsen[39] and Plyler, Danti, Blaine and Tidwell[33]. Agreement between these two investigations implies a precision of better than ±0·02 cm^{-1} and an absolute accuracy of ±0·03 cm^{-1}. Starred line 25 is resolution-sensitive. Cell length, 10 cm, p = 70 mm, t = 25°C, approximate spectral slit width, 0·4 cm^{-1}.


N₂O
580
590
600
610
620
630
WAVENUMBER
ABSORPTION
1
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13
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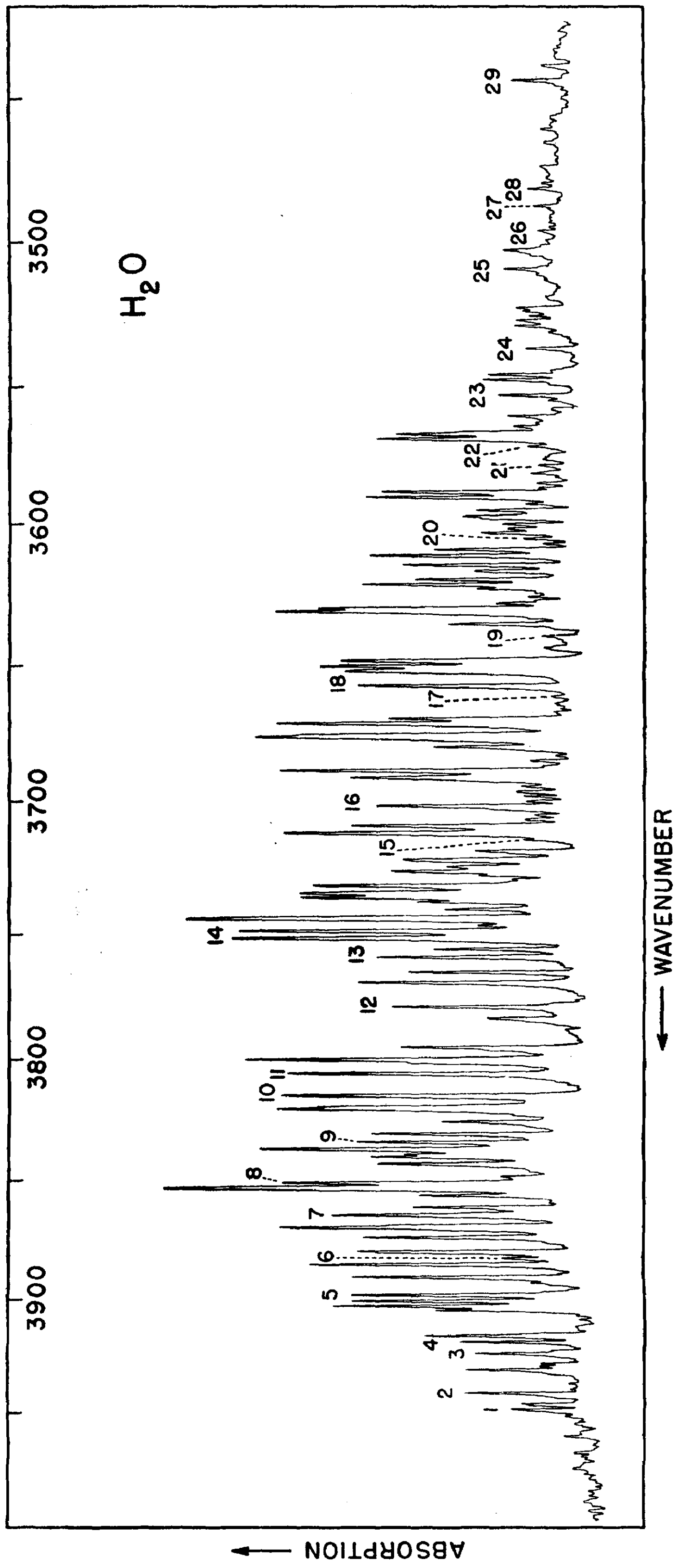
Table 18. Nitrous oxide fundamental: 630–592 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	629·29	16	616·60	31	603·91
2	628·46	17	615·74	32	603·07
3	627·61	18	614·90	33	602·23
4	626·77	19	614·06	34	601·39
5	625·93	20	613·20	35	600·54
6	625·07	21	612·35	36	599·71
7	624·22	22	611·50	37	598·87
8	623·35	23	610·65	38	598·04
9	622·53	24	609·81	39	597·22
10	621·68	25	608·98	40	596·35
11	620·84	26	608·13	41	595·52
12	619·99	27	607·29	42	594·67
13	619·14	28	606·46	43	593·82
14	618·29	29	605·61	44	592·97
15	617·44	30	604·76	45	592·13

Data from Lakshmi, Rao and Nielsen[40]. Mould, Price and Wilkinson[35] have found that the upper lines of the band tie in with those of *Table 17*, and Tidwell, Plyler and Benedict[36] have shown from the combination principle that several lines in the centre of the band are accurate to about ±0·01 cm^{-1}. A tentative absolute accuracy of ±0·02 cm^{-1} is estimated. Cell length, 10 cm, p = 300 mm, t = 25°C, approximate spectral slit width, 0·35 cm^{-1}.



H₂O
3500
3600
3700
3800
3900
2
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4
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WAVENUMBER
ABSORPTION

Table 19. Water vapour fundamentals: 3950–3447 cm^{-1}

(Virtually all lines should be starred as resolution-sensitive and not accurate to better than 0·1 cm^{-1})

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	3950·00	16	3701·90
2	3942·86	17	3659·94
3	3925·16	18	3656·30
4	3920·10	19	3638·15
5	3899·45	20	3603·08
6	3883·26	21	3577·06
7	3865·15	22	3570·54
8	3852·10	23	3552·35
9	3835·06	24	3536·44
10	3816·10	25	3509·49
11	3807·05	26	3496·63
12	3779·40	27	3488·11
13	3759·85	28	3482·28
14	3752·20	29	3447·20
15	3714·81		

Data from Plyler and Tidwell[32]. Path length through instrument open to the atmosphere, 320 cm, t = 25°C, approximate spectral slit width, 0·9 cm^{-1}. These lines are strongly pressure-sensitive and resolution-sensitive. They are not recommended for calibration purposes requiring an accuracy better than ±0·1 cm^{-1}.

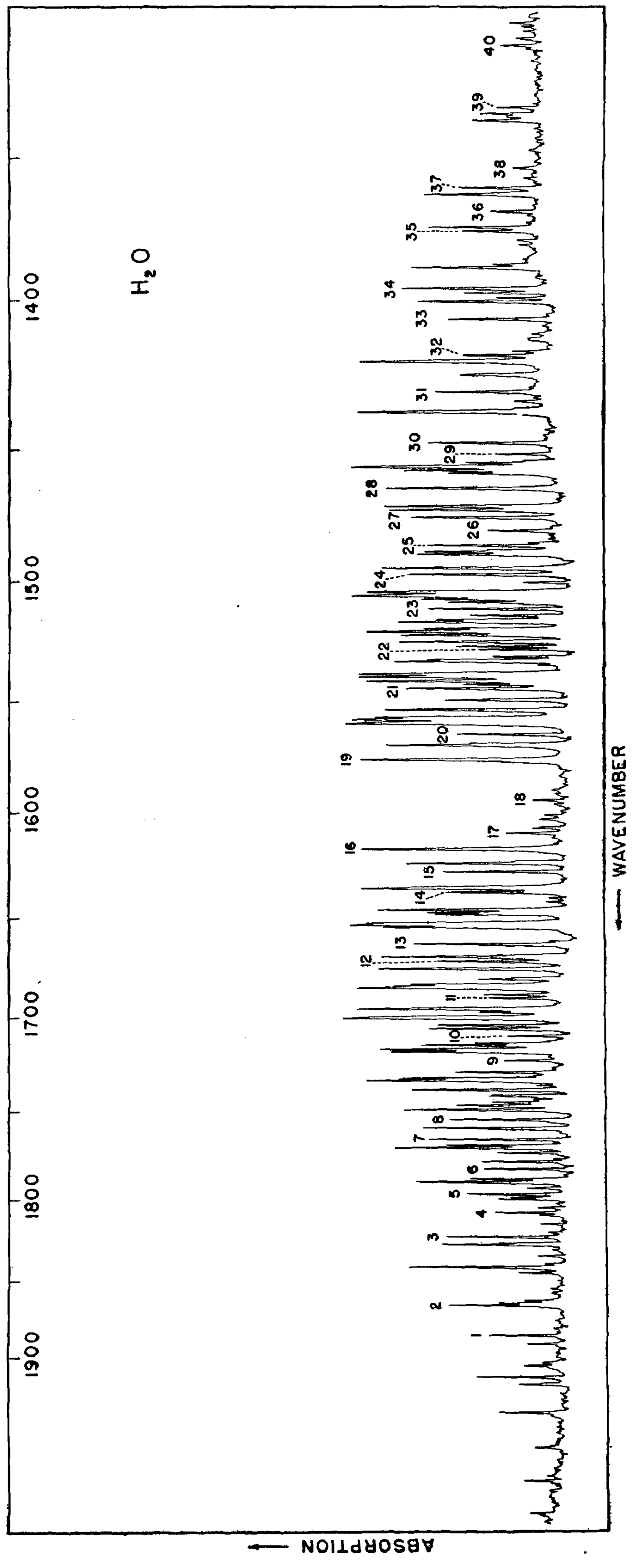
H$_2$O
1400
1500
1600
1700
1800
1900
WAVENUMBER
ABSORPTION
1
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Table 20. Water vapour fundamental: 1890–1317 cm^{-1}

Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber* (vac.) (cm^{-1})
1	1889·59	17	1609·45	33	1404·99
2	1869·36*	18	1594·51	34	1394·46*
3	1825·24	19	1576·18	35	1375·08*
4	1810·63	20	1564·87	36	1368·62
5	1799·60	21	1545·16*	37	1361·08
6	1784·95	22	1528·54*	38	1354·83
7	1768·17	23	1512·29	39	1336·62
8	1756·82	24	1498·86	40	1318·90
9	1723·48	25	1487·29		
10	1710·22	26	1481·25		
11	1690·15	27	1476·14		
12	1671·50*	28	1464·92		
13	1662·78	29	1452·06		
14	1637·53	30	1447·96		
15	1627·82	31	1429·96		
16	1616·71	32	1417·44*		

Data from Plyler, Danti, Blaine and Tidwell[33] and Rao, Ryan and Nielsen[29]. Path length through instrument open to the atmosphere, 320 cm, t = 25°C, approximate spectral slit width, 0·5 cm^{-1}. These lines are strongly pressure-sensitive and resolution-sensitive, particularly those starred. They are not recommended for calibration purposes requiring an accuracy better than ±0·1 cm^{-1}.

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PART II

WAVENUMBERS FOR THE CALIBRATION OF PRISM AND SMALL GRATING SPECTROMETERS (RESOLUTION 0·5–10 cm^{-1}) IN THE RANGE 3950–600 cm^{-1}

II. WAVENUMBERS FOR THE CALIBRATION OF PRISM AND SMALL GRATING SPECTROMETERS (RESOLUTION 0·5–10 cm^{-1}) IN THE RANGE 3950–600 cm^{-1}

INTRODUCTION

Many of the current applications of infra-red spectroscopy to the elucidation of structural and analytical problems of chemistry involve the measurement of the spectra of materials in condensed phases. Such spectra do not exhibit the rotation–vibration fine structure shown by many molecules in the vapour phase. Fine structure bands, with half-widths of less than 2 cm^{-1} occur occasionally in association with the lattice vibrations of crystals, but most solids and liquids exhibit structure-less vibration absorption bands, the half-widths of which are seldom less than 2 cm^{-1} and usually greater than 5 cm^{-1}.

In the investigation of such spectra it has been customary to employ prism spectrometers. The resolution achieved by these instruments depends on the optical design and the nature of the prism material; it may also vary widely for the same spectrometer in different regions of the spectrum. The more elaborate prism spectrometers in current use may achieve nominal spectral slit widths in the range 1–2 cm^{-1}, but they are severely energy-limited. To obtain an acceptable signal-to-noise ratio it is usually necessary to use wide slits, or else high amplifier gain combined with a narrow electrical band-pass frequency. Widening the slits leads directly to a reduction in the resolution, while decreasing the band-pass frequency causes a virtual loss of resolution and increases the instrumental distortion of the band shape. These latter effects may be partly offset by a reduction in the scanning speed, but there are practical limits to the use of such corrective measures. In view of these considerations, most prism spectrometers are operated at nominal spectral slit widths exceeding 2 cm^{-1}, and commonly in the range 2–10 cm^{-1}.

Because of their greater overall efficiency, increasing use is now being made of small grating spectrometers in the measurement of condensed phase spectra. When so used the most efficient operating conditions of the spectrometer will differ from those applicable to the measurement of vapour phase vibration–rotation spectra. The intrinsic broadness of the bands permits the use of wider slits without loss of structural detail or significant distortion of the spectrum. Optimal spectral slit widths in the range 1–2 cm^{-1} can often be used, permitting higher signal-to-noise ratios and faster scanning speeds.

The wavenumber calibration tables in Part II have been prepared by the

Commission to meet the requirements of grating spectrometers operating under these conditions, as well as prism spectrometers operating under a wide range of conditions encountered in applied chemical spectroscopy.

ARRANGEMENT OF THE TABLES

Charts 1–34

Charts 1–34 demonstrate vapour phase spectra for the wavenumber range 3950–590 cm^{-1}, each chart covers a span of 100 cm^{-1}. The same calibrant gases are used as for the Part I tables, supplemented by deuterium cyanide. The spectral ranges covered by each gas are listed on the following page. Whereas the lines listed in the corresponding tables of Part I have been chosen solely for their suitability as accurate wavenumber standards, additional factors have also been taken into consideration in the choice of the calibration lines in Part II.

Because of the intrinsic broadness of the bands in condensed-phase spectra, there is usually less need for extreme precision in the evaluation of wavenumber, and for most purposes an absolute accuracy between 0·1 and 0·5 cm^{-1} will suffice. The positions of the calibration lines listed in Part II have therefore been rounded to the nearest $0{\cdot}05_5$ cm^{-1}. This wider tolerance permits the inclusion of lines that do not meet the more critical specifications of the Part I data. In particular, it diminishes the significance of small line displacements resulting from pressure broadening, and from resolution effects on partial line overlap. Higher pressures may be used, so that bands can be followed out to higher J-numbers, and this assists materially in eliminating gaps between the ranges of different calibrant gases. Greater tolerance of small resolution-sensitive overlap effects allows the inclusion of additional lines and a more even distribution of calibration points across the spectrum. Uncertainties which may be introduced by these pressure- and resolution-sensitive displacements are compensated by a reduction in interpolation errors when instrumental scale readings are converted to wavenumber units by the methods outlined on p. 20 of Part I.

In several of the charts the wavenumber positions of closely lying doublet and triplet line groups have been recorded. These are indicated as "resolution tests" in the tables accompanying *Charts 1–34*, and are intended for the evaluation and control of spectrometer performance. Lines that appear in the tables of both Parts I and II are identified by the symbol †.

Particular features of the individual spectra which affect their use for calibration purposes are dealt with in footnotes to the individual tables, but there are a few additional matters calling for more general comment.

(*a*) *Ammonia* (*3540–3394 cm^{-1}*)—In the Part I calibration tables a gap extends from 3579 to 3386 cm^{-1} for which the Commission has been unable to locate any lines of acceptable accuracy. The ν_1 fundamental band in the spectrum of ammonia occupies this region, but the lines are highly resolution-sensitive and are judged unsuitable for high precision calibration on this account. Blends of some of these lines are included in *Charts 5* and *6* in order to provide some calibration points in this region, which is particularly important in the investigation of hydrogen bonding phenomena. For these blended lines an absolute accuracy of only $\pm 0{\cdot}2$ cm^{-1} is claimed, and it is

Summary of data for Charts 1–39
(All vapour phase spectra are measured at 10 cm path length)

Substance	*Region* (cm^{-1})	*Pressure* (mm)	*Chart no.*
Water vapour	3943–3744	sat.	1–3
Carbon dioxide	3737–3683	200	3–4
,,	3681–3591	400	4
,,	3608–3569	200	5
Ammonia	3540–3491	300	5
,,	3509–3394	75	6
Hydrogen cyanide	3399–3381	450	7
,,	3378–3245	20	7–8
,,	3231–3207	450	8
Methane	3183–3158	300	9
,,	3149–2958	60	9–11
Hydrogen chloride	3045–2624	120	10–14
Hydrogen bromide	2710–2393	140	14–17
Carbon dioxide	2386–2298	20	17
,,	2311–2292	50	18
,,	2282–2236	250	18
Carbon monoxide	2233–2055	150	18–20
Deuterium chloride	2047–1894	250	19–21
Water vapour	1943–1374	sat.	21–27
Deuterium bromide	1909–1727	60	22–23
Ammonia	1613–1580	75	24–25
Methane	1368–1266	60	27–28
,,	1260–1212	250	28
Ammonia	1213– 972	50	28–31
,,	967– 962	15	31
,,	960– 934	50	31
,,	927– 924	15	31
,,	921– 771	50	31–33
,,	761– 745	75	33
Hydrogen cyanide	786– 635	30	33–34
Acetylene	720– 694	15	33
Carbon dioxide	702– 632	70	34
Nitrous oxide	630– 593	300	34
Deuterium cyanide	630– 591	60	34
Indene	3929– 693	*	35–37
Polystyrene	3082– 699	†	38–39

* Liquid films of thickness 200 μ and 30 μ.
† Solid films of thickness 70 μ and 7 μ.

essential that in using them the resolution of the calibration spectrum be matched as closely as possible.

(*b*) *Water vapour* (*3950–3750 cm*$^{-1}$*; 1940–1370 cm*$^{-1}$)—The water vapour lines selected for inclusion in Part I are based on measurements at long path lengths (2–7 m), and some of them appear weak when observed at a path length of 10 cm of saturated water vapour at room temperature. It was considered desirable that all vapour spectra used in Part II should be based on a 10 cm path length, as the use of longer path lengths is inconvenient, particularly when working with flushed or evacuated spectrometers or when calibrating by the superposition method (Part I, p. 556). In the Part II water vapour spectra stronger lines have in some instances been selected in place of the Part I calibration lines on this account. It is of practical interest to note that the water lines are best observed with a cell containing a small amount of liquid water and thin silver chloride windows. The windows should be slightly deformed to eliminate interference patterns. The line intensities can be augmented by aspirating air or nitrogen through a water wash-bottle containing a sintered glass bubbler, and then through the cell.

On *Charts 24* and *25* the use of six lines from the spectrum of ammonia is recommended to supplement the water vapour spectrum in the region of the weak Q-branch absorption.

(*c*) *Deuterium cyanide* (*630–590 cm*$^{-1}$)—Lines from this spectrum have been added to supplement the nitrous oxide lines because the latter are too close to be resolved at spectral slit widths wider than 0·5 cm^{-1}. These data are based on the work of Checkland and Thompson (*Trans. Faraday Soc.*, **51**, 1 (1955)), and unpublished measurements of Jones.

Measurements at lower resolution; Charts 1A–34A

As the resolution of the spectrometer is diminished, the apparent half line width increases and the determination of absolute line position becomes more uncertain. It is difficult to predict the magnitude of such effects on particular groups of lines. The spectra have therefore been remeasured on a carefully calibrated grating spectrometer at a series of gradually increasing slit schedules. The lines which are least affected are distinguished by the symbol (‡) in the tables accompanying *Charts 1–34*.

These lines are also indicated on *Charts 1A–34A* and they are recommended for the calibration of prism spectrometers under conditions where the resolution of *Charts 1A–34A* can be matched or exceeded. Most of these spectra were determined at nominal spectral slit widths in the range 1·5–3 cm^{-1} which should be within the capabilities of the larger prism instruments. *Charts 3A, 4A, 5A, 17A, 18A, 33A* and *34A* were measured at nominal spectral slit widths of 1–1·5 cm^{-1}, conditions which it may be difficult to achieve with conventional prism spectrometers under routine operating conditions. The accuracy of the line positions under the conditions of *Charts 1A–34A* should not differ greatly from that reported in the tables; an increase in tolerance by a factor of two might reasonably be allowed. On the broader lines the major uncertainty will lie in the evaluation of the position of the curve maximum.

Charts 35–39; liquid and solid phase calibrant materials for small prism spectrometers

The smaller types of prism spectrometers are difficult to calibrate from vapour phase spectra because their low dispersion does not resolve a sufficient number of calibration lines, and the interpolation errors become increasingly large. This is true particularly where a sodium chloride prism is utilized above 2000 cm^{-1}.

Interpolation techniques for dealing with this situation have been proposed by McKinney and Friedel (*J. Opt. Soc. Am.*, **38**, 222 (1948)), and by Bethke (*J. Opt. Soc. Am.*, **46**, 560 (1956)). Their use, with specific applications to various categories of prism spectrometers, has been outlined by Downie, Magoon, Purcell and Crawford (*J. Opt. Soc. Am.*, **43**, 941 (1956)). Because of limitations inherent in the optical and mechanical design of these smaller instruments, it is unlikely that spectrometers of this type will be capable of a precision better than ±1 cm^{-1} through most regions of the spectrum, and it is more convenient, and probably no less accurate, to calibrate with carefully measured vibrational bands from the spectra of selected liquids and solids.

It is the view of the Commission that more extensive measurements of this kind are desirable to provide a wider range of liquid and solid phase spectra suitable for this purpose. In *Charts 35–39* the spectra of liquid indene and of a polystyrene film are reproduced. The provisional band positions listed in the accompanying tables are taken from the data of Jones, Jonathan, Nadeau and MacKenzie (*Spectrochim. Acta*, in press) for indene and of Plyler, Danti, Blaine and Tidwell (*J. Research Natl. Bur. Standards*, **64**, 29 (1960)), and Jones and Nadeau (unpublished) for polystyrene.

Collectively these spectra provide approximately one hundred provisional calibration points, most of which should be within the resolution capabilities of the small prism spectrometers under consideration. These data should allow calibration of such instruments with a precision of ±1 cm^{-1} providing spectral slit widths of 10 cm^{-1} or less can be achieved.

Preparation of gaseous samples

The majority of the gases are readily obtained from commercial sources. Deuterium chloride is conveniently prepared by the drop-wise action of deuterium oxide on phosphorus pentachloride at room temperature. Deuterium bromide is similarly obtainable from deuterium oxide and phosphorus tribromide with gentle warming. Deuterium cyanide can be prepared by the action of dideutero-sulphuric acid on potassium cyanide, or alternatively from phosphorus pentoxide, deuterium oxide and potassium cyanide as described by Richardson (*J. Phys. Chem.*, **19**, 1213 (1951)).

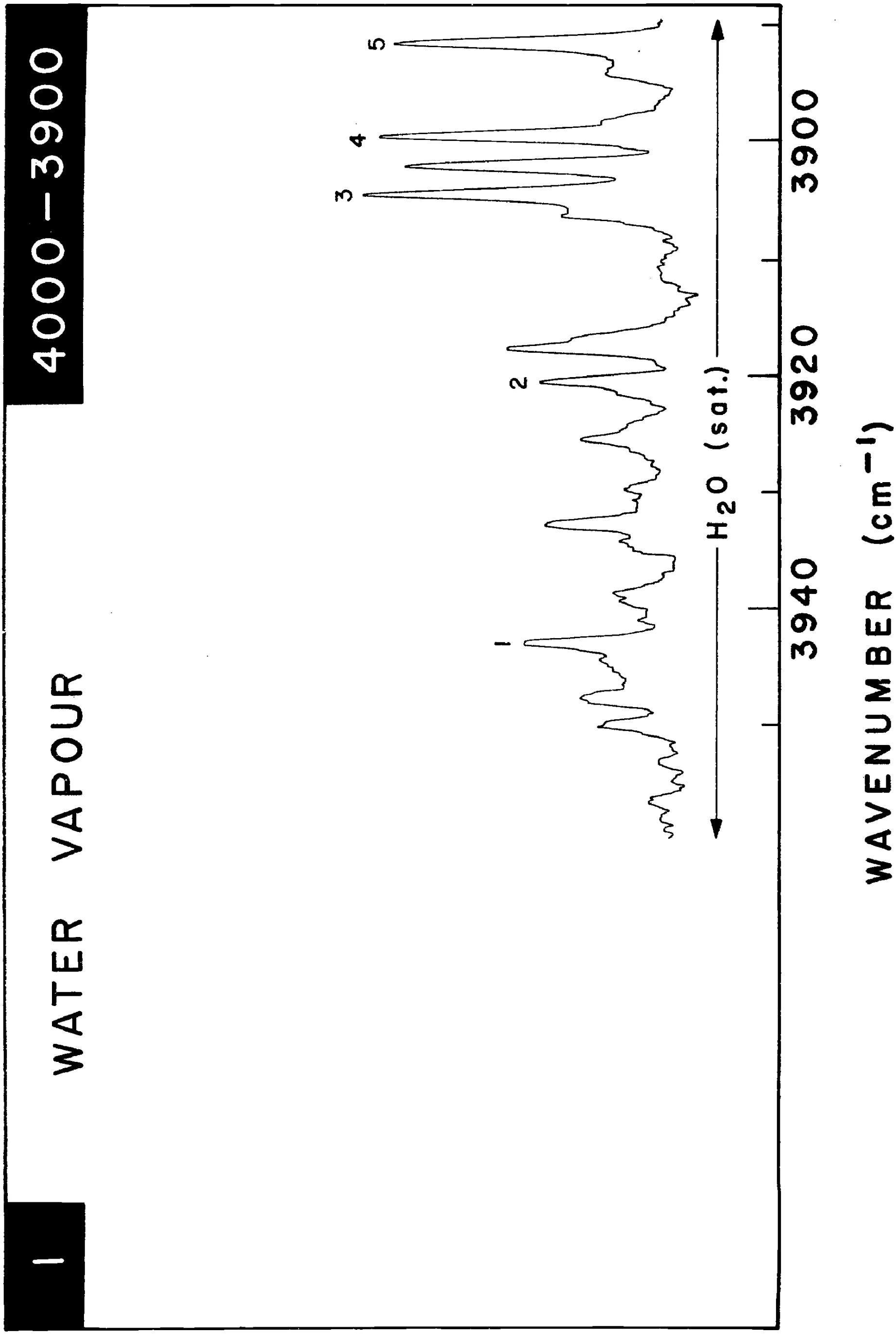
I
WATER VAPOUR
4000 – 3900
1
2
3
4
5
H_2O (sat.)
3940
3920
3900
WAVENUMBER (cm^{-1})

Chart 1. Water vapour (saturated): 3950–3900 cm^{-1}

Line no.	*Wavenumber*[a, b] (vac.) (cm^{-1})
1	3942·8$_5$†‡
2	3920·1†
3	3904·2$_5$
4	3899·4$_5$†
5	3891·3‡

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 1A*).
(a) Most of these lines are blends and will resolve under higher resolution (Part I).
(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

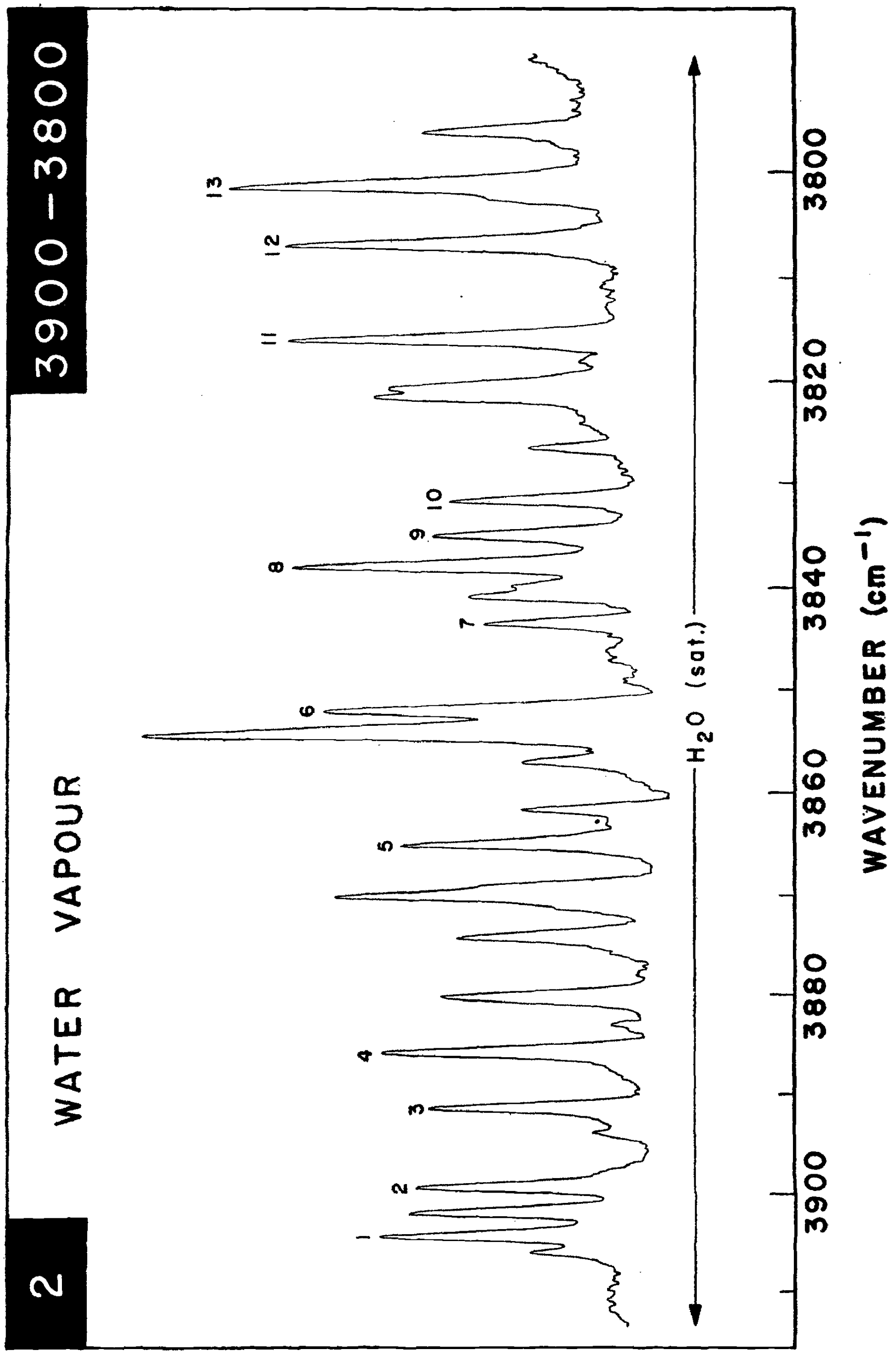
2
3900 – 3800
WATER VAPOUR
1
2
3
4
5
6
7
8
9
10
11
12
13
H_2O (sat.)
3900
3880
3860
3840
3820
3800
WAVENUMBER (cm^{-1})

Chart 2. Water vapour (saturated): 3900–3800 cm^{-1}

Line no.	*Wavenumber*[a,b] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[a,b] (vac.) (cm^{-1})
1	3904·2$_5$	7	3843·8
2	3899·4$_5$†	8	3837·9‡
3	3891·3‡	9	3835·0$_5$†
4	3885·9‡	10	3831·7‡
5	3865·1$_5$†‡	11	3816·1†‡
6	3852·1†	12	3807·0$_5$†‡
		13	3801·4‡

Resolution tests: Line no. 8–line no. 9: 2·85 cm^{-1}
Line no. 9–line no. 10: 3·35 cm^{-1}

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† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 2A*).
(a) Most of these lines are blends and will resolve under higher resolution (Part I).
(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

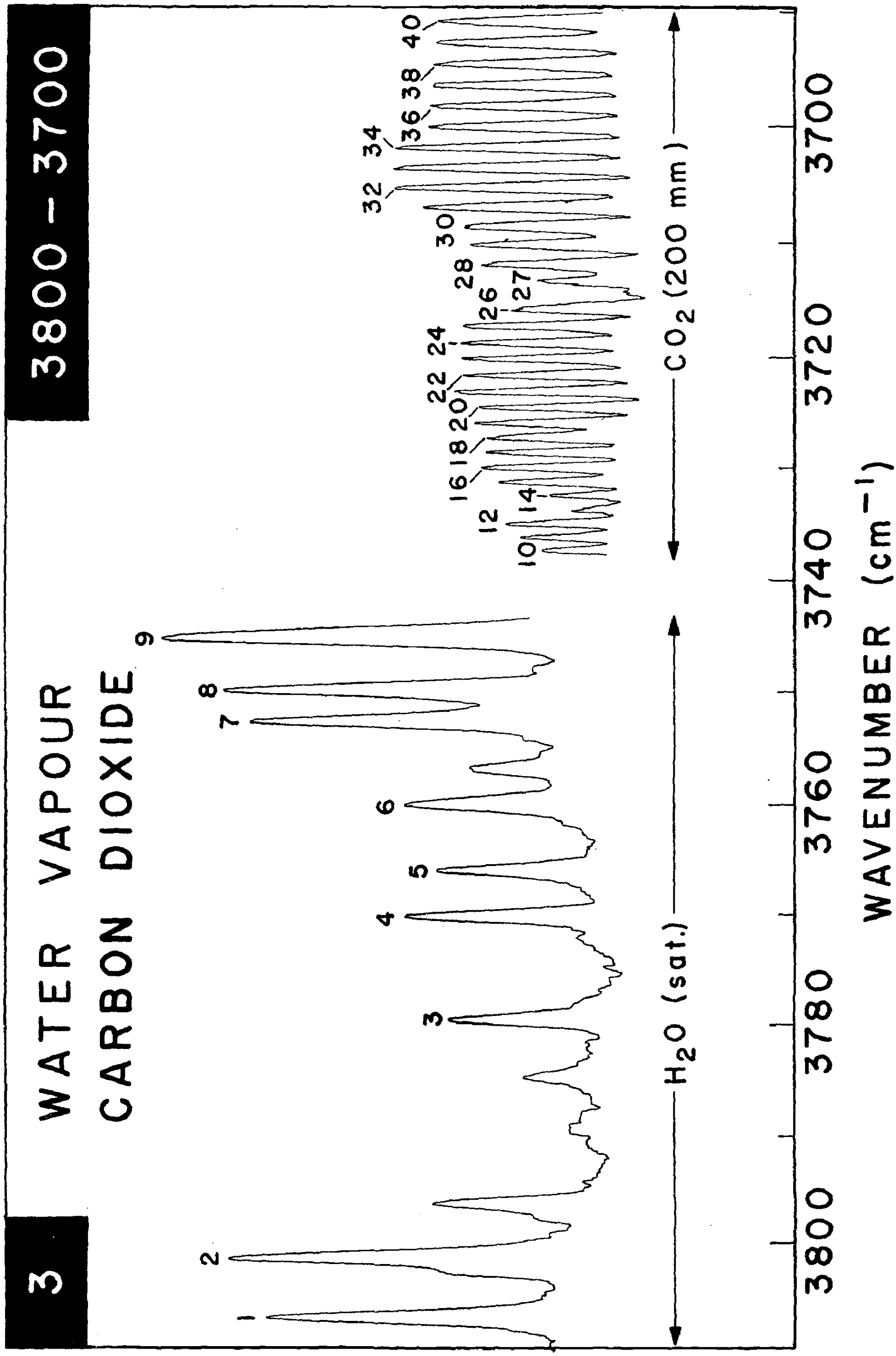
3
3800 – 3700
WATER VAPOUR
CARBON DIOXIDE
1
2
3
4
5
6
7
8
9
10
12
14
16
18
20
22
24
26
27
28
30
32
34
36
38
40
H_2O (sat.)
CO_2 (200 mm)
3800
3780
3760
3740
3720
3700
WAVENUMBER (cm^{-1})

Chart 3. Water vapour (saturated) and carbon dioxide (200 mm): 3800–3700 cm^{-1}

Line no.	*Water vapour (saturated)* *Wavenumber*$^{(a,b)}$ (vac.) (cm^{-1})	Line no.	*Carbon dioxide* (200 mm) *Wavenumber*$^{(b)}$ (vac.) (cm^{-1})	Line no.	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})
1	3807·0$_5$†‡	10	3737·0	25	3717·1‡
2	3801·4‡	11	3735·8$_5$	26	3715·5$_5$
3	3779·4†	12	3734·7	27	3713·2
4	3769·8‡	13	3733·5†	28	3711·6$_5$
5	3765·8	14	3732·2	29	3710·0
6	3759·8$_5$†‡	15	3731·0†	30	3708·4†
7	3752·2†‡	16	3729·7$_5$†	31	3706·7†‡
8	3749·3‡	17	3728·4†	32	3705·0†‡
9	3744·5‡	18	3727·0$_5$‡	33	3703·3†‡
		19	3725·7†	34	3701·5$_5$‡
		20	3724·3$_5$†	35	3699·8†‡
		21	3722·9†‡	36	3698·0†‡
		22	3721·5‡	37	3696·1$_5$‡
		23	3720·1†‡	38	3694·3$_5$†‡
		24	3718·6‡	39	3692·4$_5$†‡
				40	3690·5$_5$‡

Resolution tests: Line no. 16–line no. 17: 1·35 cm^{-1}
Line no. 32–line no. 33: 1·7 cm^{-1}
Line no. 7–line no. 8: 2·9 cm^{-1}

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† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 3A*); where the dispersion is insufficient to resolve these lines, the line at 3701·9 cm^{-1} in the spectrum of water vapour may be employed as a calibration point.

(a) Most of these lines are blends and will resolve under higher resolution (Part I).

(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

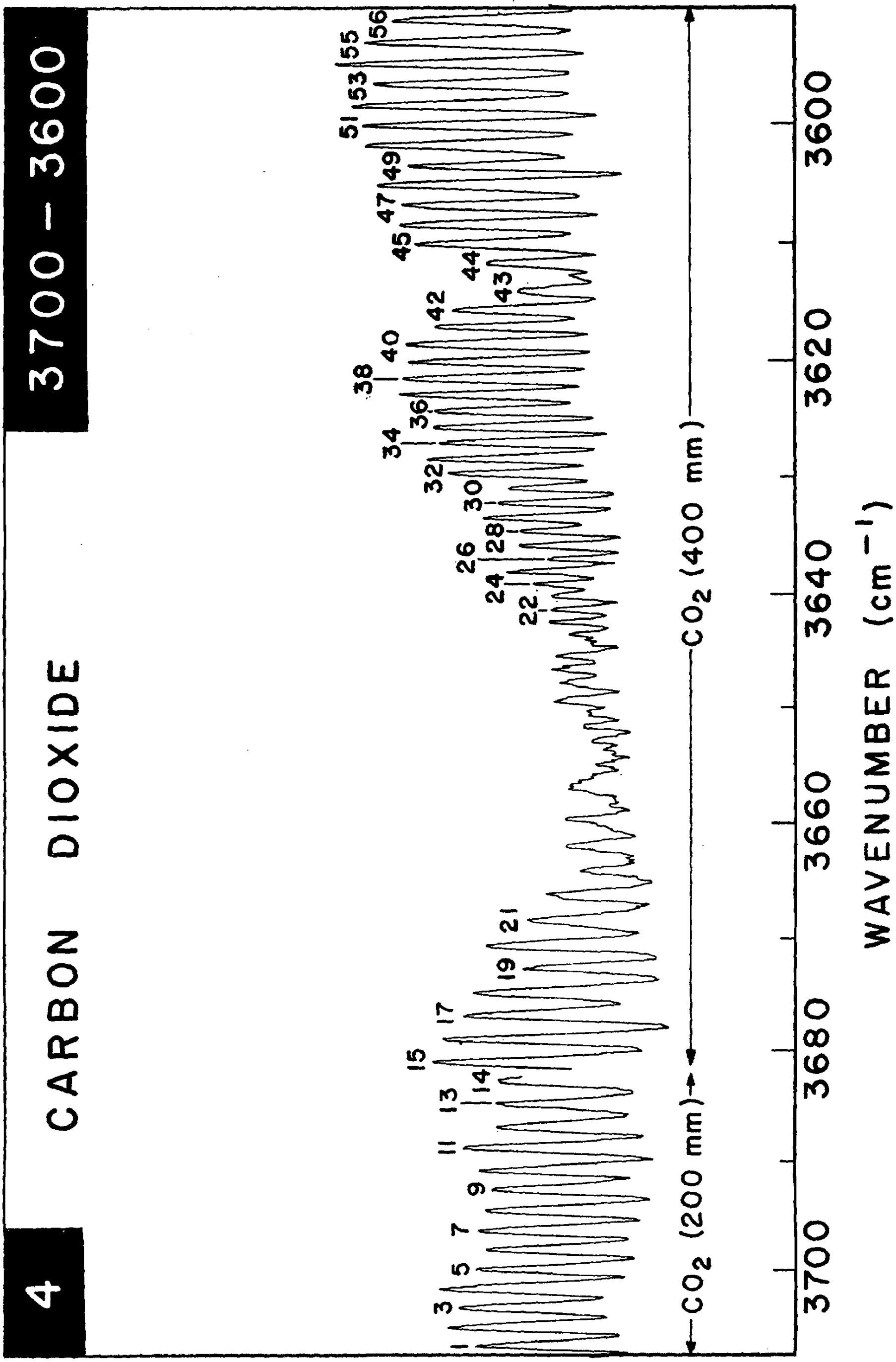
4
CARBON DIOXIDE
3700 – 3600
1
3
5
7
9
11
13
14
15
17
19
21
22
24
26
28
30
32
34
36
38
40
42
43
44
45
47
49
51
53
55
56
CO₂ (200 mm)
CO₂ (400 mm)
3700
3680
3660
3640
3620
3600
WAVENUMBER (cm⁻¹)

Chart 4. Carbon dioxide (200 mm) and (400 mm): 3700–3600 cm^{-1}

Carbon dioxide (200 mm)		*Carbon dioxide* (400 mm)			
Line no.	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})
1	3706·7†‡	15	3680·7$_5$‡	36	3623·9$_5$†‡
2	3705·0†‡	16	3678·7‡	37	3622·5†‡
3	3703·3†‡	17	3676·6$_5$	38	3621·1$_5$†‡
4	3701·5$_5$‡	18	3674·6	39	3619·6‡
5	3699·8†‡	19	3672·5	40	3618·1$_5$‡
6	3698·0†‡	20	3670·3$_5$‡	41	3616·6$_5$‡
7	3696·1$_5$‡	21	3668·2‡	42	3615·2$_5$†‡
8	3694·3$_5$†‡	22	3641·1	43	3613·6
9	3692·4$_5$	23	3640·0†	44	3611·3
10	3690·5$_5$‡	24	3638·9$_5$	45	3609·7‡
11	3688·6$_5$‡	25	3637·8	46	3608·0$_5$†‡
12	3686·7$_5$†‡	26	3636·6$_5$	47	3606·5†‡
13	3684·7$_5$‡	27	3635·5	48	3604·8†‡
14	3682·8†‡	28	3634·3	49	3603·1‡
		29	3633·0$_5$	50	3601·4†‡
		30	3631·8$_5$†	51	3599·7$_5$†‡
		31	3630·5$_5$	52	3598·0$_5$‡
		32	3629·3	53	3596·2†‡
		33	3628·0	54	3594·4†‡
		34	3626·6	55	3592·6$_5$†‡
		35	3625·2$_5$†	56	3590·8†‡

Resolution tests: Line no. 34–line no. 35: 1·35 cm^{-1}
Line no. 51–line no. 52: 1·75 cm^{-1}
Line no. 7–line no. 8: 1·80 cm^{-1}

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† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 4A*); where the dispersion is insufficient to resolve these lines, the lines at 3701·9 and 3656·3 cm^{-1} in the spectrum of water vapour may be employed as calibration points.

(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

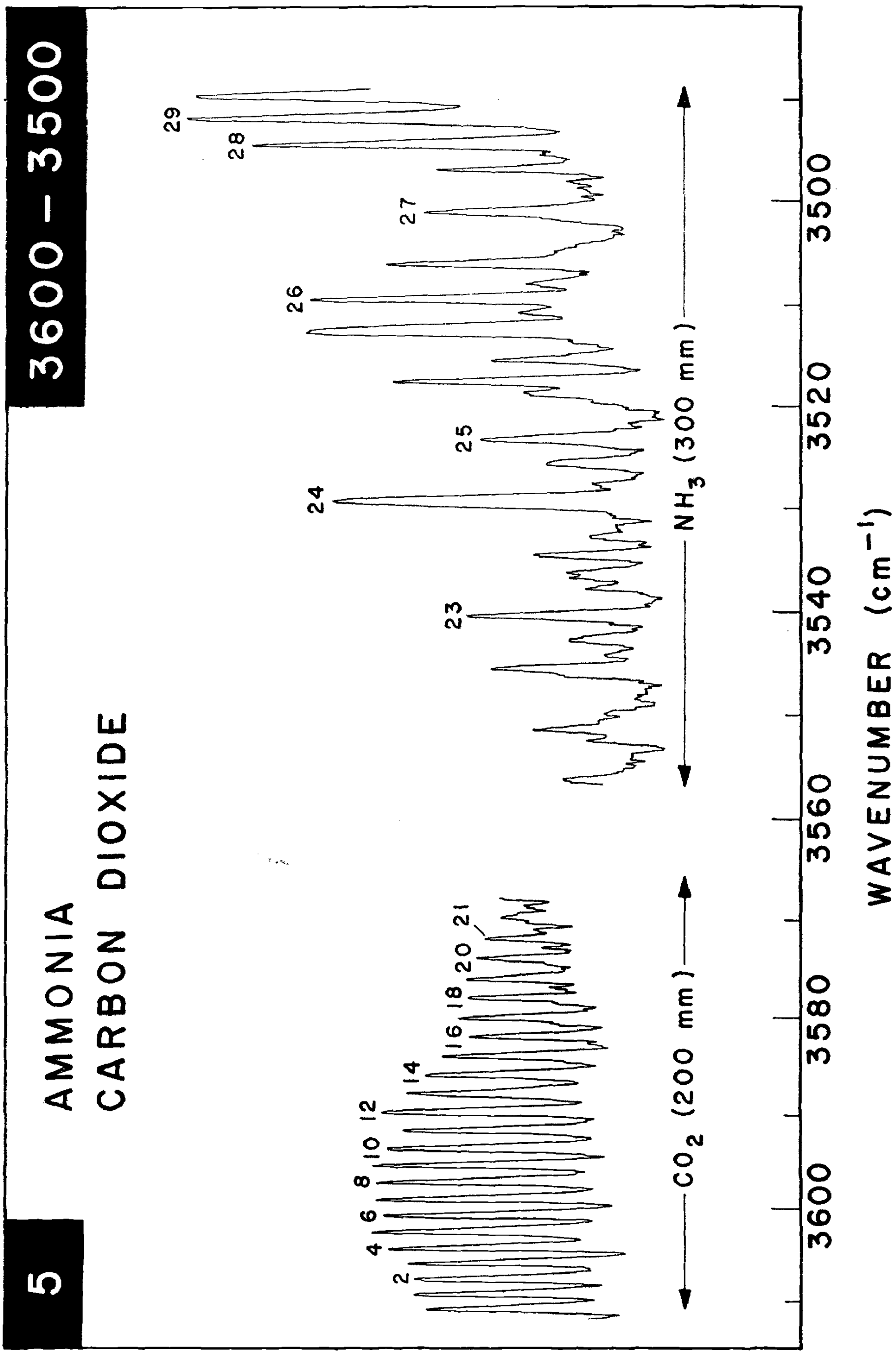
5
3600 – 3500
AMMONIA
CARBON DIOXIDE
2
4
6
8
10
12
14
16
18
20
21
23
24
25
26
27
28
29
CO$_2$ (200 mm)
NH$_3$ (300 mm)
3600
3580
3560
3540
3520
3500
WAVENUMBER (cm^{-1})

Chart 5. Carbon dioxide (200 mm) and ammonia (300 mm): 3600–3500 cm^{-1}

Carbon dioxide (200 mm)		*Ammonia* (300 mm)			
Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(b c) (vac.) (cm^{-1})
1	3608·0$_5$‡	12	3588·9$_5$‡	23	3540·1
2	3606·5†‡	13	3587·1‡	24	3529·0‡
3	3604·8†‡	14	3585·2†‡	25	3523·1‡
4	3603·1$_5$‡	15	3583·2$_5$‡	26	3508·9$_5$‡
5	3601·4†‡	16	3581·3†‡	27	3500·4‡
6	3599·7$_5$†‡	17	3579·3$_5$†‡	28	3493·9‡
7	3598·0‡	18	3577·3$_5$‡	29	3491·4
8	3596·2†‡	19	3575·4		
9	3594·4†‡	20	3573·4		
10	3592·6$_5$†‡	21	3571·3		
11	3590·8†‡	22	3569·2		

Resolution tests: Line no. 9–line no. 10: 1·75 cm^{-1}
Line no. 28–line no. 29: 2·5 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 5A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) The estimated uncertainty is ±0·2 cm^{-1}.
(c) These lines are all blends and should not be used for calibration if the resolution exceeds that shown in *Chart 5*.

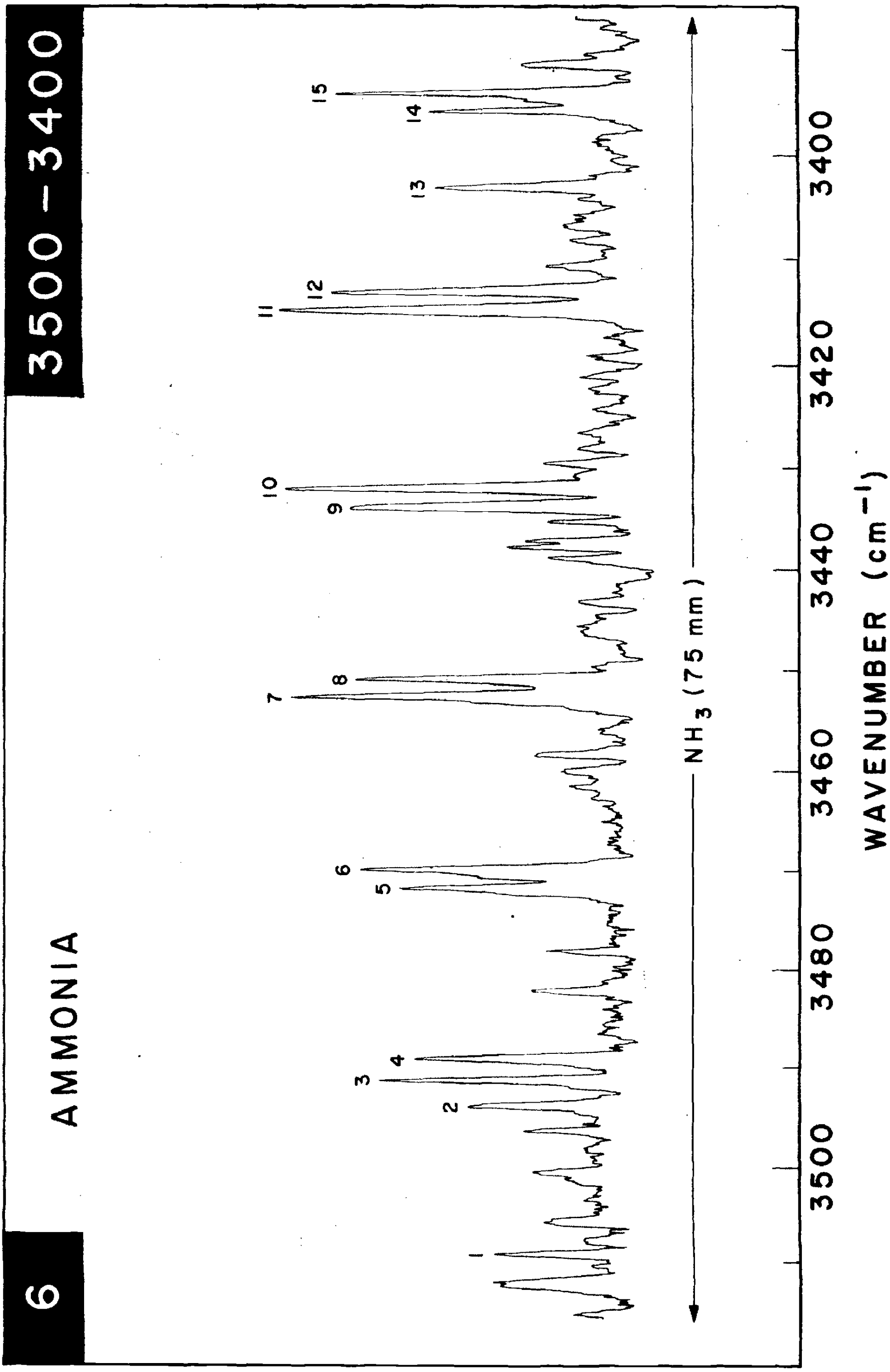
6
AMMONIA
3500 – 3400
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
NH_3 (75 mm)
3500
3480
3460
3440
3420
3400
WAVENUMBER (cm^{-1})

Chart 6. Ammonia (75 mm): 3500–3400 cm^{-1}

Line no.	*Wavenumber*‡(a,b) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*‡(a,b) (vac.) (cm^{-1})
1	$3508{\cdot}9_5$	9	3433·8
2	3493·9	10	3432·0
3	3491·4	11	3414·7
4	3489·3	12	3413·1
5	3471·7	13	3403·1‡
6	3469·8	14	$3395{\cdot}6_5$
7	3452·7	15	3393·9
8	3450·9		

Resolution tests: Line no. 7–line no. 8: 1·8 cm^{-1}

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‡ Under lower resolution (*Chart 6A*) only line no. 13 remains as an acceptable calibration point. The blended lines no. 5/6, 7/8, 9/10, 11/12, and 14/15 have peaks at 3470·4 cm^{-1}, 3452·1 cm^{-1}, 3432·6 cm^{-1}, 3414·1 cm^{-1}, and 3394·5 cm^{-1} under the conditions shown in *Chart 6A*. These values can be used for calibration purposes to ±0·5 cm^{-1}.

(a) These lines are all blends and should not be used for calibration if the resolution exceeds that shown in *Chart 6*.

(b) The estimated uncertainty is ±0·2 cm^{-1}.

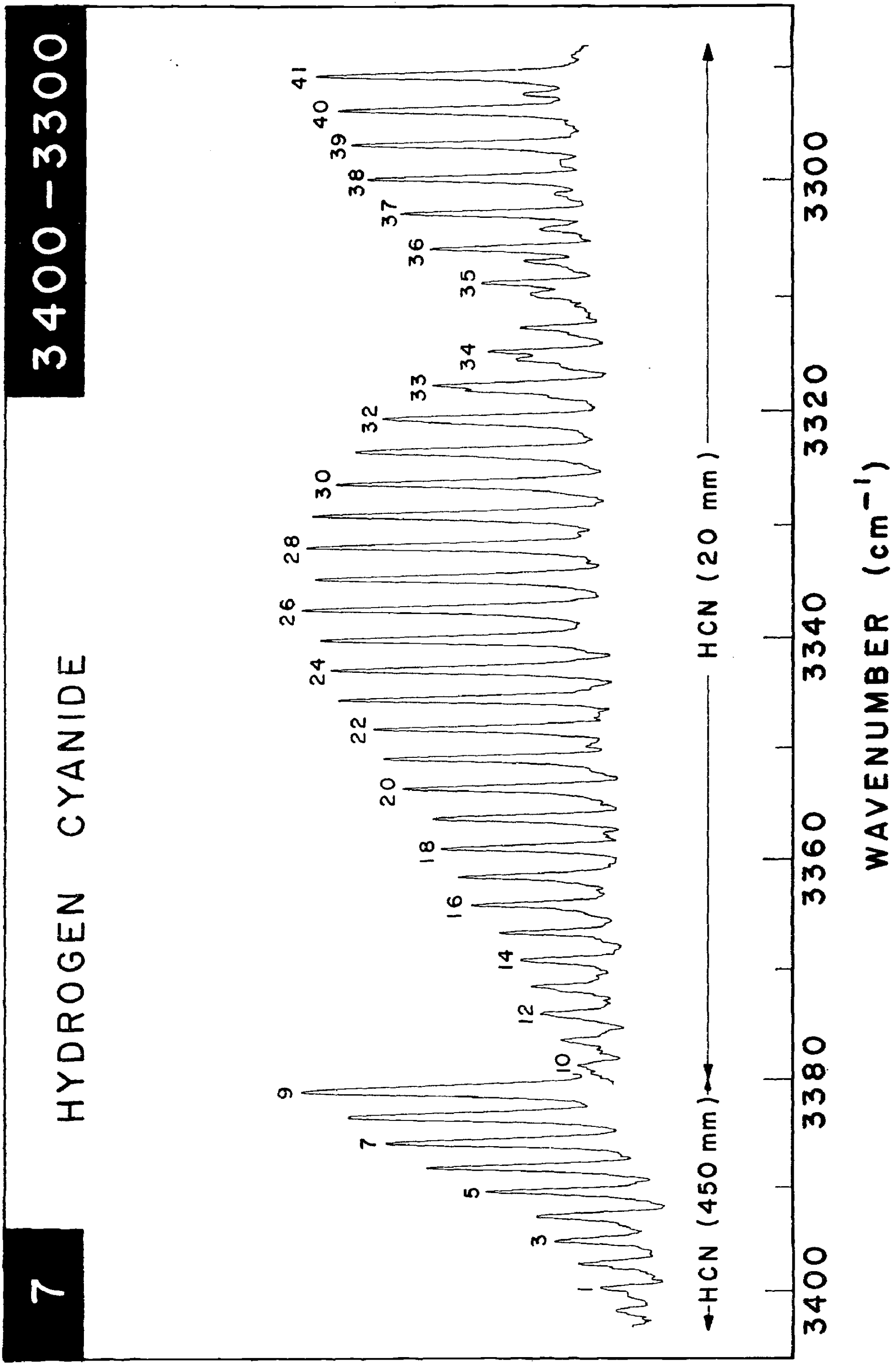
7
HYDROGEN CYANIDE
3400 – 3300
1
3
5
7
9
10
12
14
16
18
20
22
24
26
28
30
32
33
34
35
36
37
38
39
40
41
HCN (450 mm)
HCN (20 mm)
3400
3380
3360
3340
3320
3300
WAVENUMBER (cm^{-1})

Chart 7. Hydrogen cyanide (450 mm) and (20 mm): 3400–3300 cm^{-1}

Hydrogen cyanide (450 mm) *Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})	*Hydrogen cyanide* (20 mm) *Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	3399·1$_5$	10	3378·4$_5$†	26	3337·1$_5$†‡
2	3396·9$_5$	11	3376·0†	27	3334·3$_5$†‡
3	3394·7	12	3373·6†	28	3331·6†‡
4	3392·4$_5$	13	3371·1†	29	3328·8†‡
5	3390·2	14	3368·6$_5$†	30	3325·9$_5$†‡
6	3387·9	15	3366·1$_5$†	31	3323·1†‡
7	3385·5$_5$†	16	3363·6†	32	3320·2†‡
8	3383·2†	17	3361·0$_5$†	33	3317·3‡
9	3380·8$_5$†	18	3358·5†	34	3314·4
		19	3355·9†	35	3308·5†
		20	3353·3†	36	3305·5$_5$†
		21	3350·6$_5$†‡	37	3302·5$_5$†
		22	3348·0†‡	38	3299·5†‡
		23	3345·3†‡	39	3296·5†‡
		24	3342·6†‡	40	3293·4†‡
		25	3339·9†‡	41	3290·3$_5$†‡

Resolution tests: Line no. 7–line no. 8: 2·35 cm^{-1}
Line no. 25–line no. 26: 2·75 cm^{-1}
Line no. 39–line no. 40: 3·1 cm^{-1}

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† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 7A*); the unresolved ammonia line complex at 3394·5 ±0·5 cm^{-1} may also be employed (*Chart 6A*).

(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

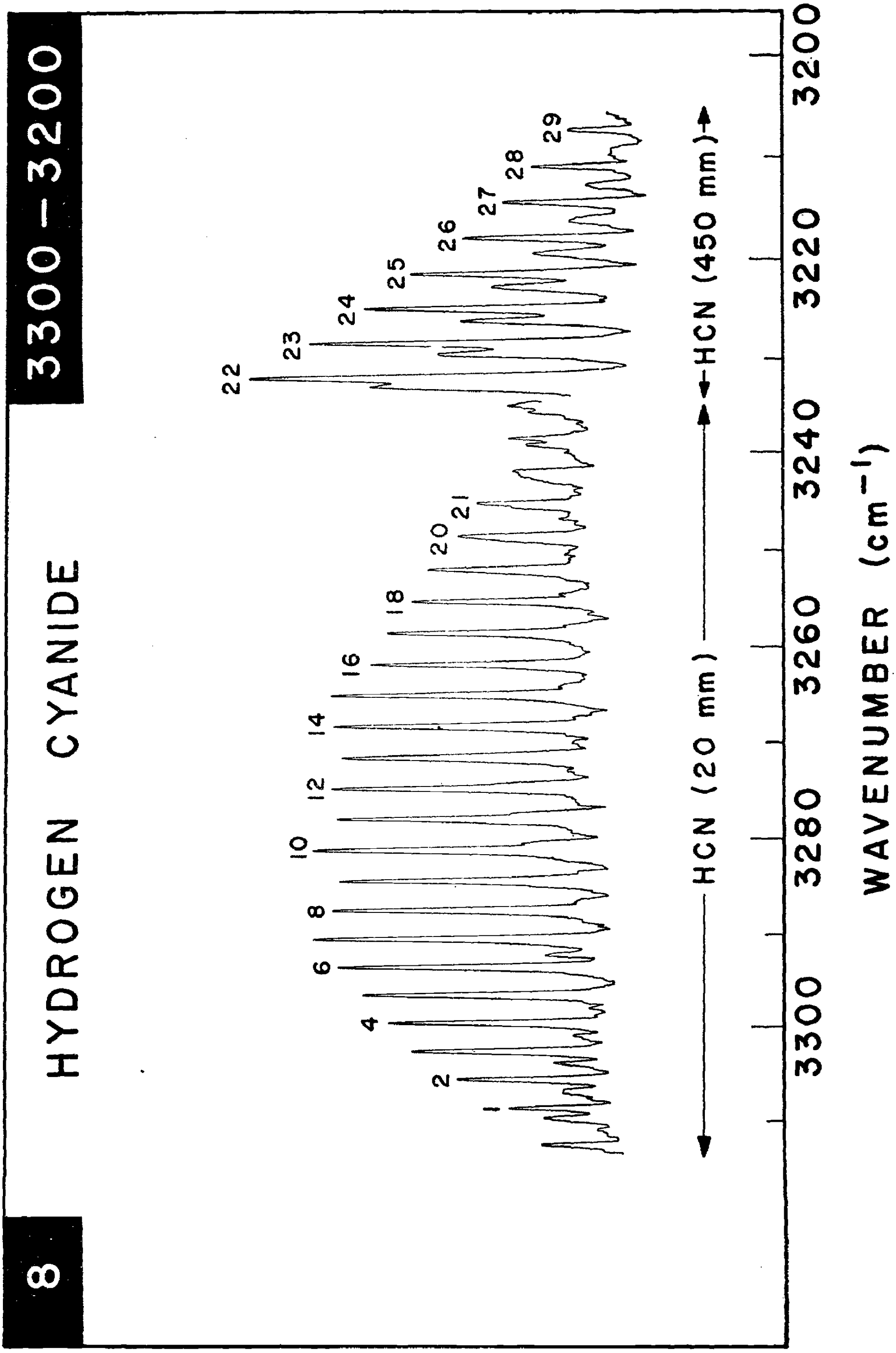

8
HYDROGEN CYANIDE
3300 – 3200
1
2
4
6
8
10
12
14
16
18
20
21
22
23
24
25
26
27
28
29
HCN (20 mm)
HCN (450 mm)
3300
3280
3260
3240
3220
3200
WAVENUMBER (cm^{-1})

Chart 8. Hydrogen cyanide (20 mm) and (450 mm): 3300–3200 cm^{-1}

Hydrogen cyanide (20 mm)				Hydrogen cyanide (450 mm)	
Line no.	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})
1	3308·5†	13	3271·4$_5$†‡	22	3231·5
2	3305·5$_5$†	14	3268·2†‡	23	3228·0$_5$
3	3302·5$_5$†	15	3265·0†‡	24	3224·6
4	3299·5†‡	16	3261·7†‡	25	3221·1
5	3296·5†‡	17	3258·4$_5$†‡	26	3217·6
6	3293·4†‡	18	3255·1$_5$†‡	27	3214·0$_5$
7	3290·3$_5$†‡	19	3251·8†‡	28	3210·5
8	3287·2$_5$†‡	20	3248·5†‡	29	3206·9$_5$
9	3284·1†‡	21	3245·1†‡		
10	3281·0†‡				
11	3277·8†‡				
12	3274·6$_5$†‡				

Resolution tests: Line no. 10–line no. 11: 3·2 cm^{-1}
Line no. 26–line no. 27: 3·55 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 8A*).

(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

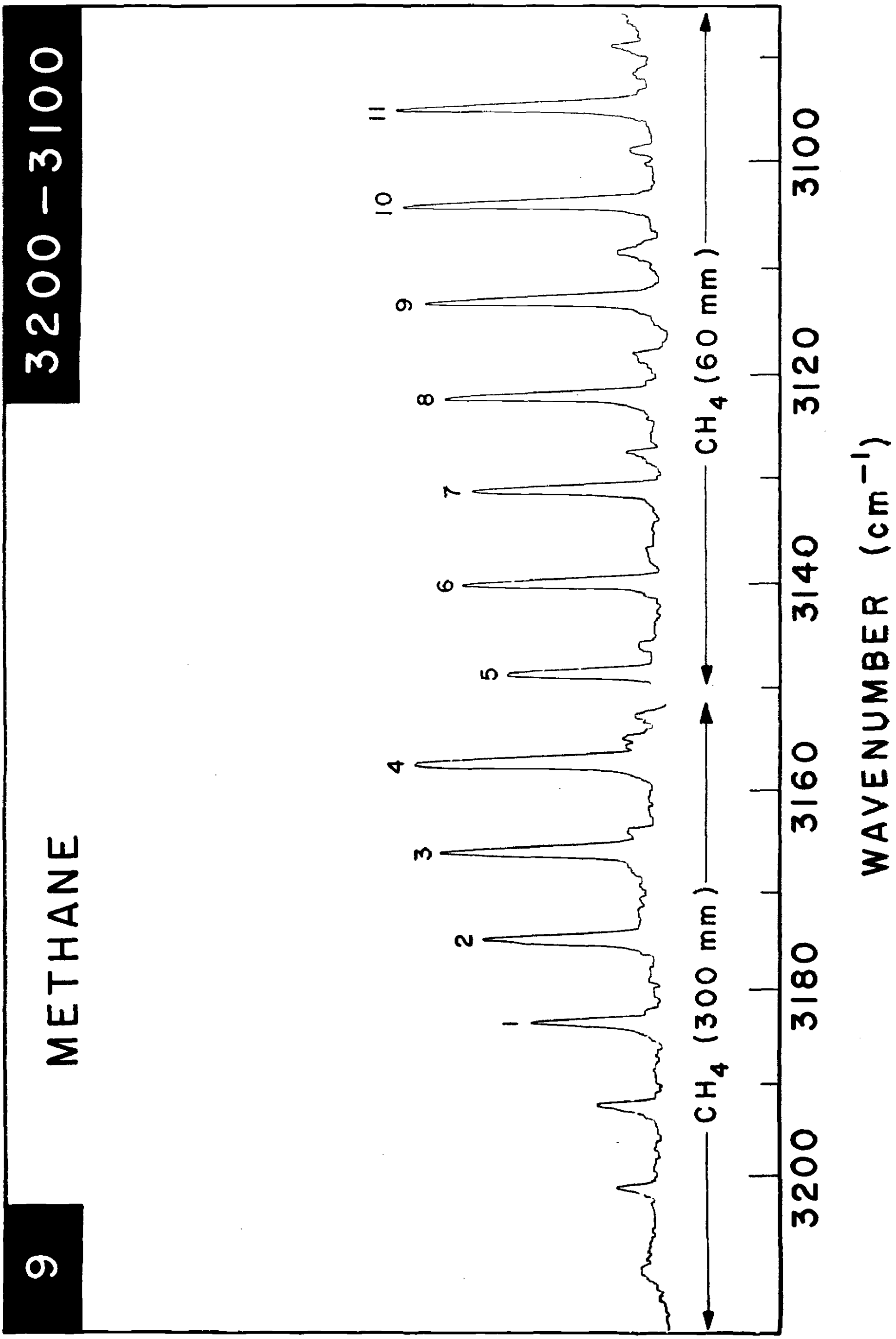

9
METHANE
3200 — 3100
1
2
3
4
5
6
7
8
9
10
11
CH_4 (300 mm)
CH_4 (60 mm)
3200
3180
3160
3140
3120
3100
WAVENUMBER (cm^{-1})

Chart 9. Methane (300 mm) and (60 mm): 3200–3100 cm^{-1}

Methane (300 mm)		*Methane* (60 mm)	
Line no.	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})
1	3183·1	5	$3148{\cdot}9_5$†‡
2	$3174{\cdot}8_5$	6	3140·2†‡
3	3166·2†‡	7	3131·4†‡
4	3157·6†‡	8	$3122{\cdot}4_5$†‡
		9	3113·4†‡
		10	$3104{\cdot}3_5$†‡
		11	3095·2†‡

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 9A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

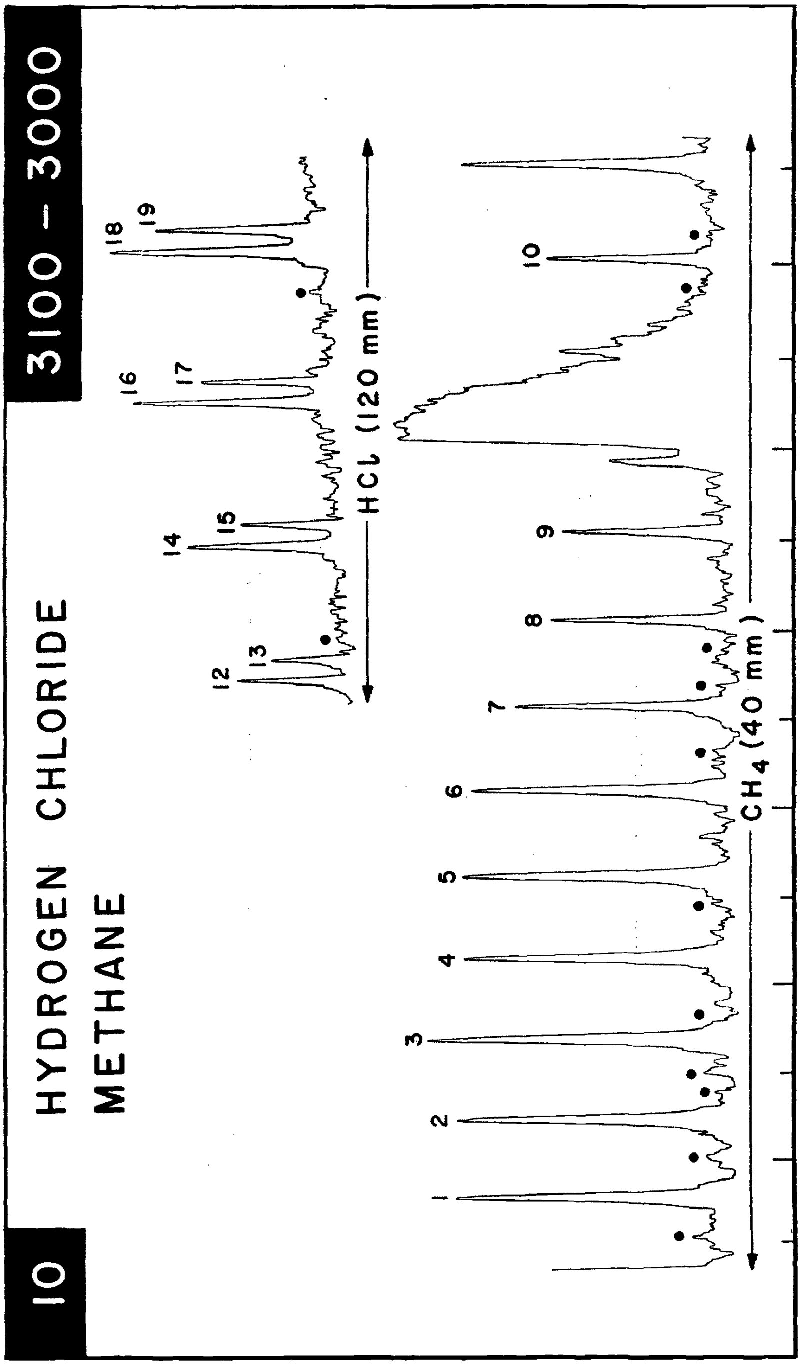

10
3100 – 3000
HYDROGEN CHLORIDE
METHANE
HCL (120 mm)
CH₄ (40 mm)
1
2
3
4
5
6
7
8
9
10
12
13
14
15
16
17
18
19
3100
3080
3060
3040
3020
3000
WAVENUMBER (cm⁻¹)

Chart 10. Methane (40 mm) and hydrogen chloride (120 mm): 3100–3000 cm^{-1}

	Methane (40 mm)		*Hydrogen chloride* (120 mm)		
Line no.	*Wavenumber*(a,c) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a,b,c) (vac.) (cm^{-1})		
1	3104·3$_5$†‡	12	3045·0$_5$†‡	(3044·5)	(±0·3 cm^{-1})
2	3095·2†‡	13	3042·7$_5$†		
3	3086·0†‡	14	3030·1†‡	(3029·5)	(±0·3 cm^{-1})
4	3076·7$_5$†‡	15	3027·8†		
5	3067·3†‡	16	3014·4$_5$†‡	(3013·8$_5$)	(±0·3 cm^{-1})
6	3057·8†‡	17	3012·1$_5$†		
7	3048·2$_5$†‡	18	2998·0$_5$†‡	(2997·5)	(±0·3 cm^{-1})
8	3038·6†‡	19	2995·8†		
9	3028·8$_5$†‡				
10	2999·1†‡				

Resolution test: Line no. 16–line no. 17: 2·3 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 10A*).

(a) **Black circles on charts indicate positions of prominent water vapour lines.**

(b) Under lower resolution the position of the more intense ($H^{35}Cl$) peak of each doublet is not significantly displaced provided the two peaks are separately resolved, as shown in *Charts 10A–14A*. If the resolution is further diminished, so that the lines blend, the main peak is displaced to lower wavenumber. If the blended line appears symmetrical, the position of the peak corresponds approximately to the weighted average of the positions of the two component lines, based on the $^{35}Cl/^{37}Cl$ abundance ratio of 0·75. These values are given in parentheses in the tables accompanying *Charts 10–14*.

(c) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

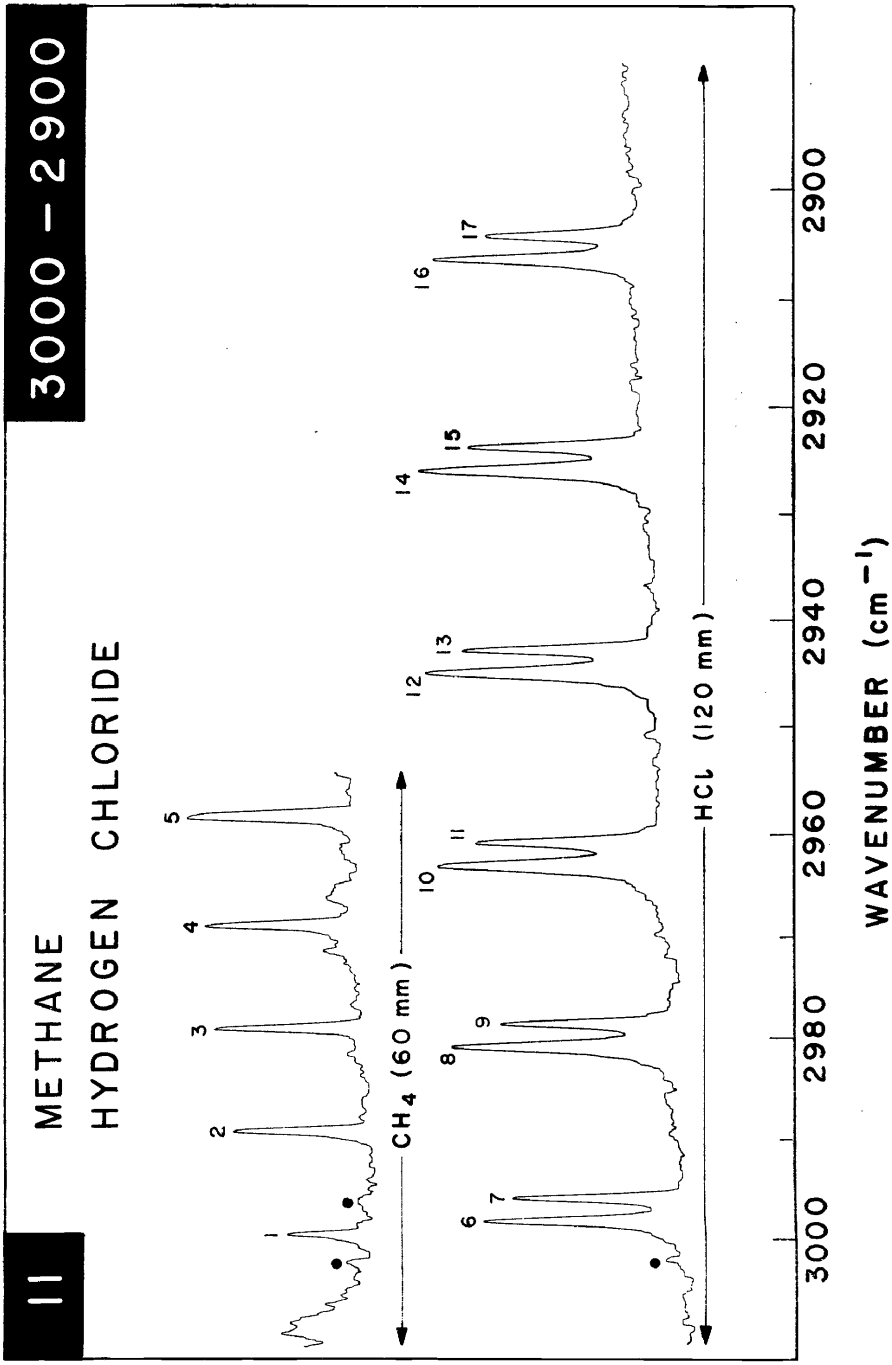

11
3000 – 2900
METHANE
HYDROGEN CHLORIDE
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
CH₄ (60 mm)
HCl (120 mm)
3000
2980
2960
2940
2920
2900
WAVENUMBER (cm⁻¹)

Chart 11. Methane (60 mm) and hydrogen chloride (120 mm): 3000–2900 cm^{-1}

Methane (60 mm)		*Hydrogen Chloride* (120 mm)			
Line no.	*Wavenumber*$^{(b,c)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a,b,c)}$ (vac.) (cm^{-1})		
1	2999·1†‡	6	2998·0$_5$†‡	(2997·5)	(±0·3 cm^{-1})
2	2989·0†‡	7	2995·8†		
3	2979·0†‡	8	2981·0†‡	(2980·4$_5$)	(±0·3 cm^{-1})
4	2968·6$_5$†‡	9	2978·7$_5$†		
5	2958·2†‡	10	2963·3†‡	(2962·7$_5$)	(±0·3 cm^{-1})
		11	2961·1†		
		12	2944·9$_5$†‡	(2944·4)	(±0·3 cm^{-1})
		13	2942·7$_5$†		
		14	2925·9†‡	(2925·3$_5$)	(±0·3 cm^{-1})
		15	2923·7$_5$†		
		16	2906·2$_5$†‡	(2905·7$_5$)	(±0·3 cm^{-1})
		17	2904·1$_5$†		

Resolution tests: Line no. 16–line no. 17: 2·1 cm^{-1}
Line no. 6–line no. 7: 2·25 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 11A*), see also footnote (b) to *Chart 10.*

(a) See footnote (b) to *Chart 10.*

(b) Black circles indicate positions of prominent atmospheric water vapour lines.

(c) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

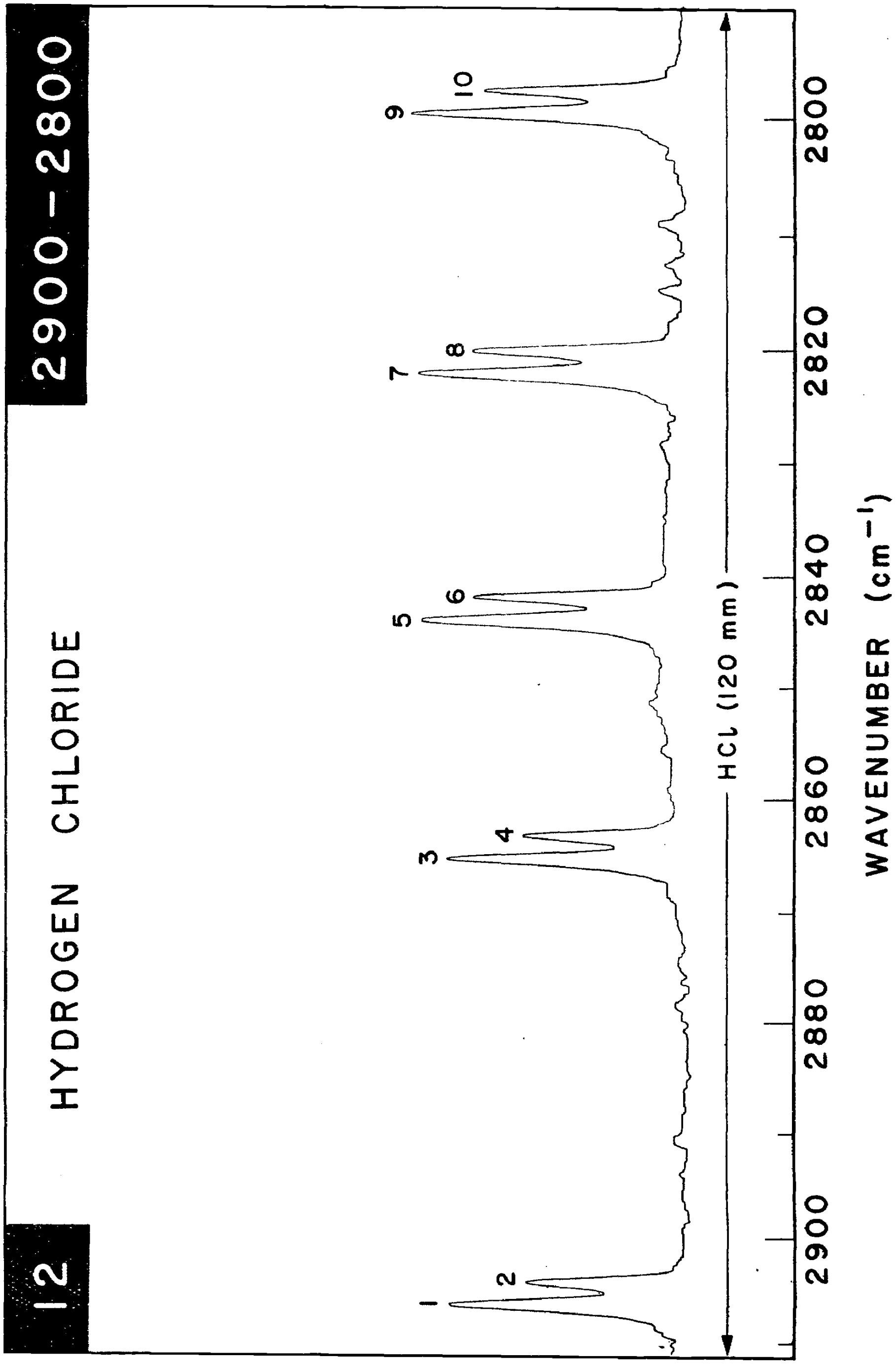

12
HYDROGEN CHLORIDE
2900 – 2800
1
2
3
4
5
6
7
8
9
10
HCL (120 mm)
2900
2880
2860
2840
2820
2800
WAVENUMBER (cm⁻¹)

Chart 12. Hydrogen chloride (120 mm): 2900–2800 cm^{-1}

Line no.	*Wavenumber*[a, b] (vac.) (cm^{-1})		
1	2906·2$_5$†‡	(2905·7$_5$)	(±0·3 cm^{-1})
2	2904·1$_5$†		
3	2865·1†‡	(2864·6)	(±0·3 cm^{-1})
4	2863·0$_5$†		
5	2843·6$_5$†‡	(2843·1$_5$)	(±0·3 cm^{-1})
6	2841·6†		
7	2821·6†‡	(2821·1)	(±0·3 cm^{-1})
8	2819·6†		
9	2798·9$_5$†‡	(2798·4$_5$)	(±0·3 cm^{-1})
10	2797·0†		

Resolution tests: Line no. 9–line no. 10: 1·95 cm^{-1}
Line no. 1–line no. 2: 2·1 cm^{-1}

---

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 12A*), see also footnote (b) to *Chart 10.*
(a) See footnote (b) to *Chart 10.*
(b) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

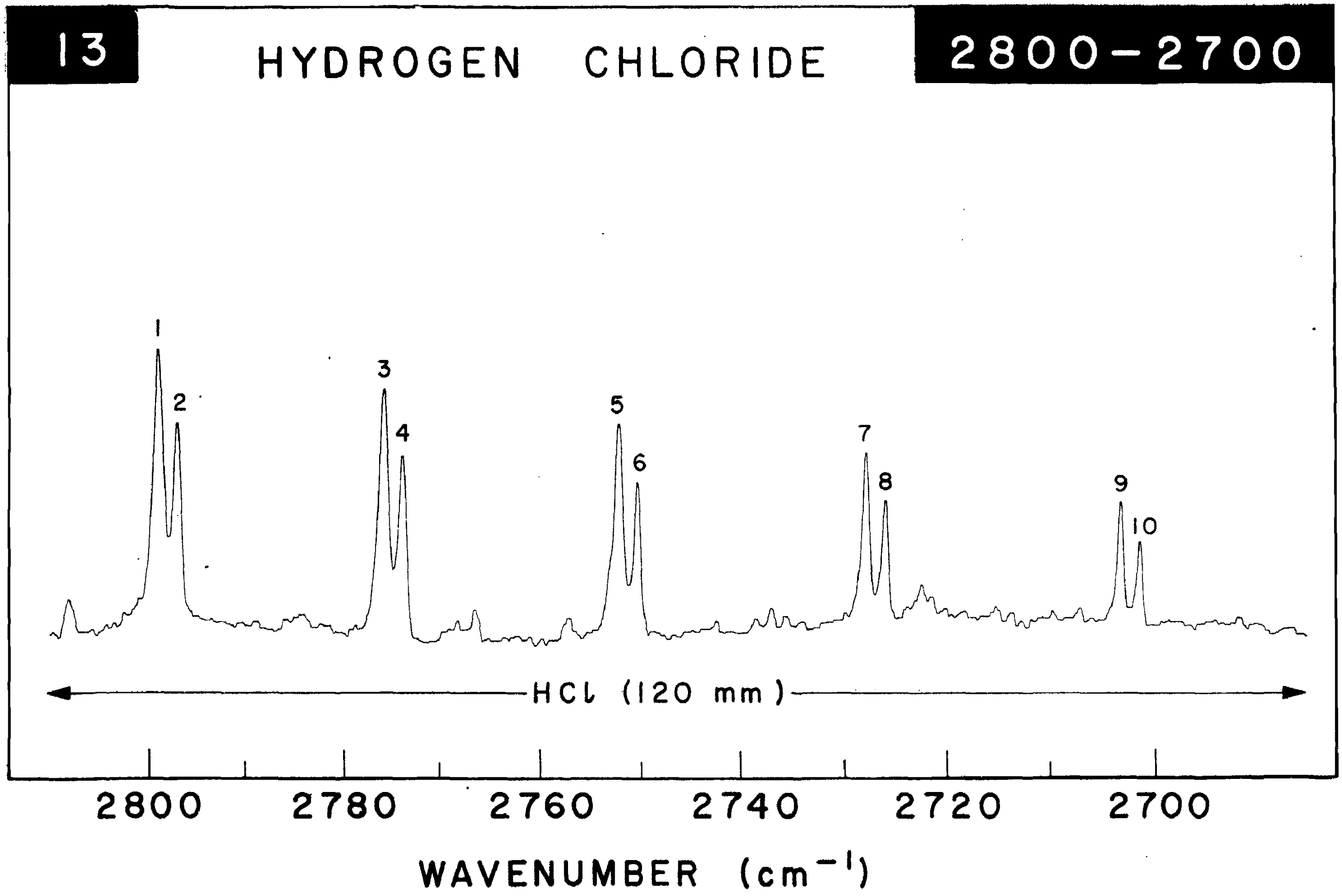

13
HYDROGEN CHLORIDE
2800–2700
1
2
3
4
5
6
7
8
9
10
HCl (120 mm)
2800
2780
2760
2740
2720
2700
WAVENUMBER (cm^{-1})

Chart 13. Hydrogen chloride (120 mm): 2800–2700 cm^{-1}

Line no.	*Wavenumber*$^{(a, b)}$ (vac.) (cm^{-1})		
1	2798·9$_5$†‡	(2798·4$_5$)	(±0·3 cm^{-1})
2	2797·0†		
3	2775·8†‡	(2775·3)	(±0·3 cm^{-1})
4	2773·8$_5$†		
5	2752·0$_5$†‡	(2751·6)	(±0·3 cm^{-1})
6	2750·1$_5$†		
7	2727·8†‡	(2727·3$_5$)	(±0·3 cm^{-1})
8	2725·9$_5$†		
9	2703·0$_5$†‡	(2702·6)	(±0·3 cm^{-1})
10	2701·2†		

Resolution tests: Line no. 9–line no. 10: 1·85 cm^{-1}
Line no. 1–line no. 2: 1·95 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 13A*), see also footnote (b) to *Chart 10.*

(a) See footnote (b) to *Chart 10.*

(b) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

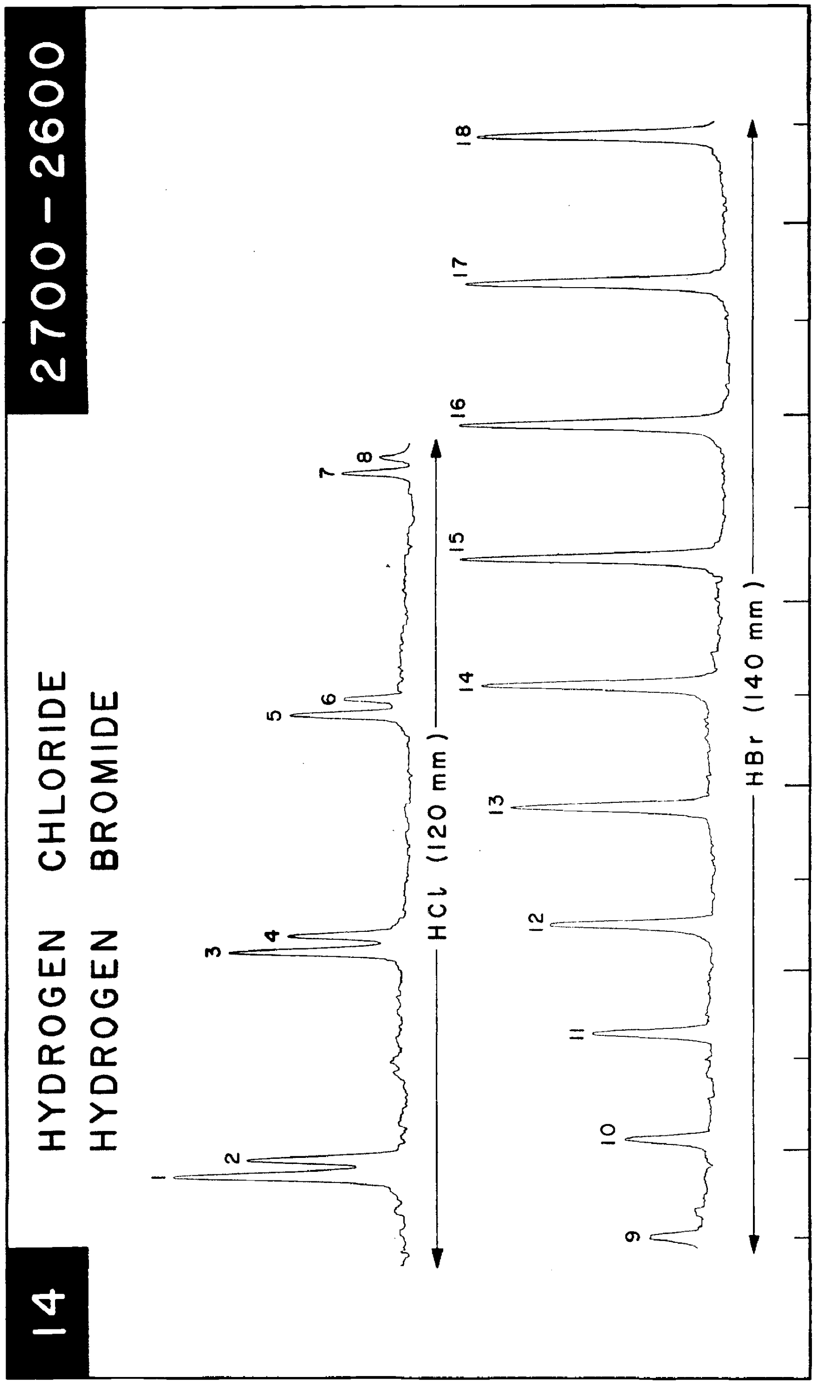

14
2700 - 2600
HYDROGEN CHLORIDE
HYDROGEN BROMIDE
1
2
3
4
5
6
7
8
HCl (120 mm)
9
10
11
12
13
14
15
16
17
18
HBr (140 mm)
2700
2680
2660
2640
2620
2600
WAVENUMBER (cm^{-1})

Chart 14. Hydrogen chloride (120 mm) and hydrogen bromide (140 mm): 2700–2600 cm^{-1}

	Hydrogen chloride (120 mm)		*Hydrogen bromide* (140 mm)	
Line no.	*Wavenumber*$^{(a, b)}$ (vac.) (cm^{-1})		*Line no.*	*Wavenumber*$^{(b, c)}$ (vac.) (cm^{-1})
1	2703·0$_5$†‡	(2702·5$_5$)($\pm$0·3 cm^{-1})	9	2710·0$_5$†‡
2	2701·2†		10	2698·9†‡
3	2677·7$_5$†‡	(2677·3)($\pm$0·3 cm^{-1})	11	2687·2†‡
4	2675·9$_5$†		12	2674·9$_5$†‡
5	2652·0†‡	(2651·5$_5$)($\pm$0·3 cm^{-1})	13	2662·2†‡
6	2650·2$_5$†		14	2648·9†‡
7	2625·7	—	15	2635·1†‡
8	2624·0		16	2620·8†‡
			17	2606·0$_5$†‡
			18	2590·7$_5$†‡
Resolution tests:	Line no. 18 unresolved doublet spacing is 0·39 cm^{-1} Line no. 12 unresolved doublet spacing is 0·40 cm^{-1} Line no. 7–line no. 8: 1·7 cm^{-1} Line no. 1–line no. 2: 1·85 cm^{-1}			

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 14A*), see also footnote (b) to *Chart 10*.

(a) See footnote (b) to *Chart 10*.

(b) The estimated uncertainty does not exceed $\pm$0·1 cm^{-1} unless otherwise indicated.

(c) The lines are blends of two components from H^{35}Br and H^{37}Br. Where the doublet is resolved the data from *Table 8* of Part I should be used.

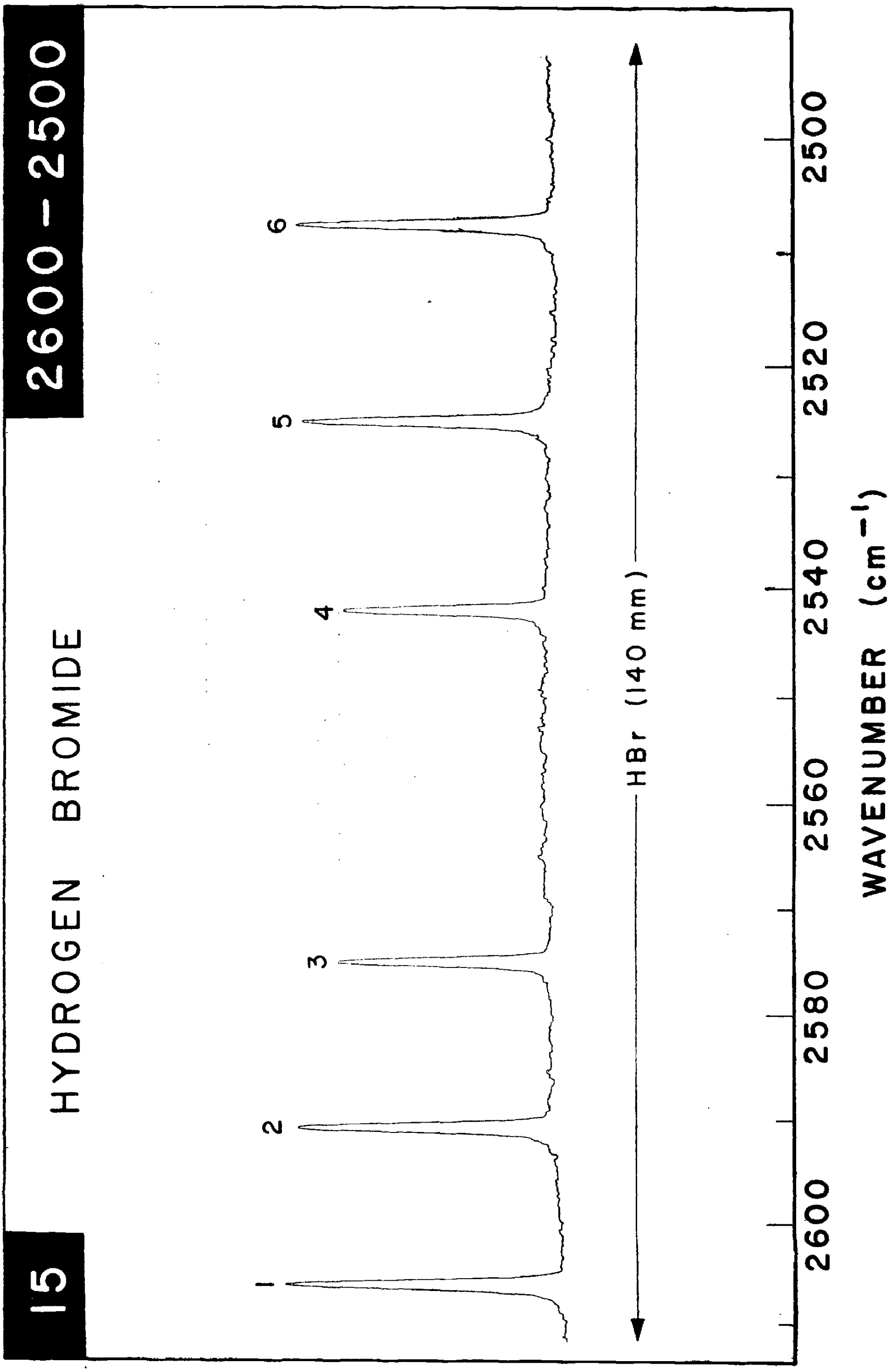

15
2600 - 2500
HYDROGEN BROMIDE
1
2
3
4
5
6
HBr (140 mm)
2600
2580
2560
2540
2520
2500
WAVENUMBER (cm⁻¹)

Chart 15. Hydrogen bromide (140 mm): 2600–2500 cm^{-1}

Line no.	*Wavenumber*$^{(a,b)}$ (vac.) (cm^{-1})
1	$2606{\cdot}0_5$†‡
2	$2590{\cdot}7_5$†‡
3	2575·0†‡
4	$2542{\cdot}0_5$†‡
5	2524·9†‡
6	2507·3†‡

Resolution tests: Line no. 6 unresolved doublet spacing is 0·36 cm^{-1}
Line no. 1 unresolved doublet spacing is 0·40 cm^{-1}

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 15A*).

(a) These lines are blends of two components from $H^{79}Br$ and $H^{81}Br$. Where the doublet is resolved the data from *Table 8* of Part I should be used.

(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

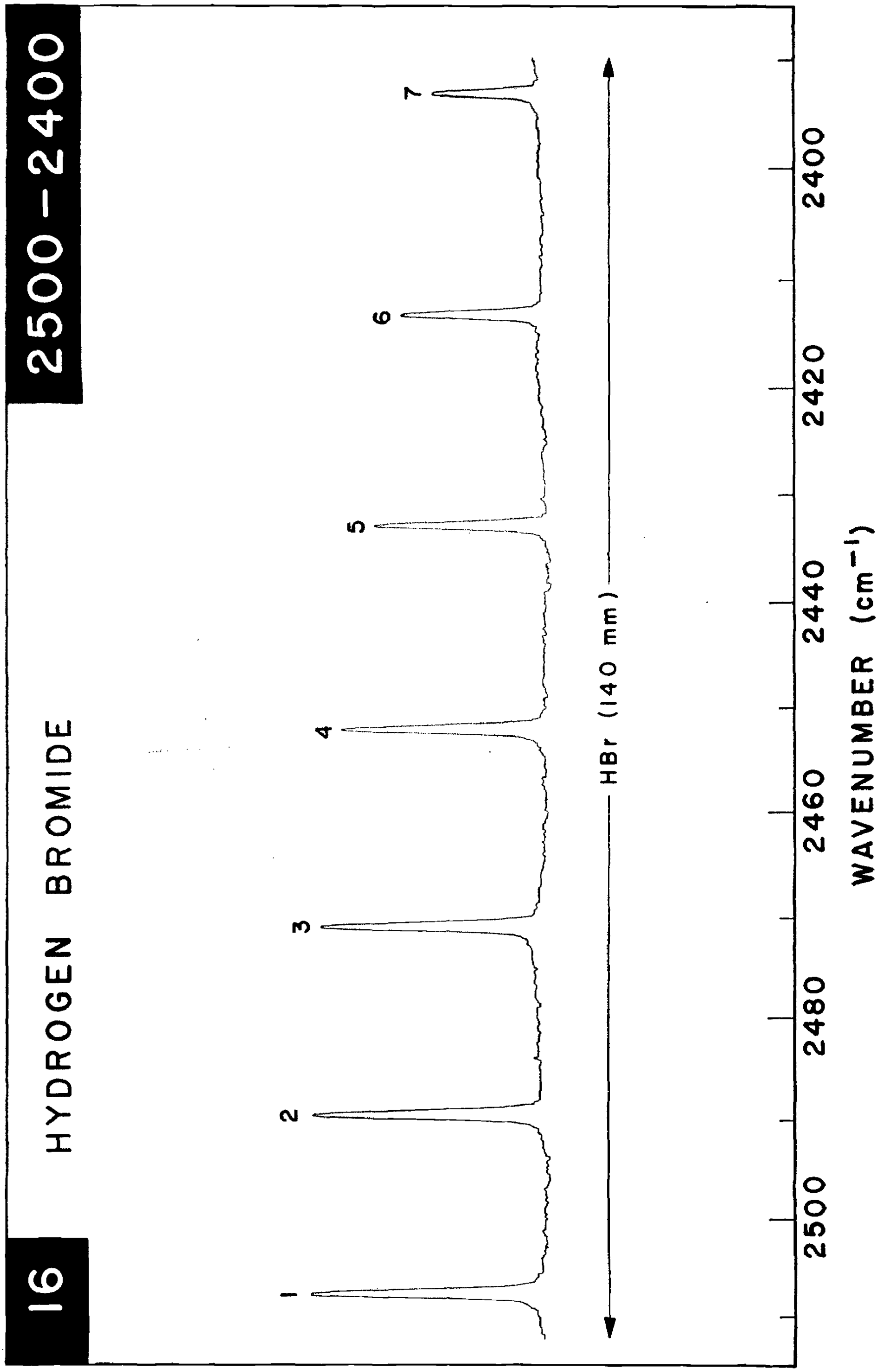

16
HYDROGEN BROMIDE
2500 – 2400
1
2
3
4
5
6
7
HBr (140 mm)
2500
2480
2460
2440
2420
2400
WAVENUMBER (cm^{-1})

Chart 16. Hydrogen bromide (140 mm): 2500–2400 cm^{-1}

Line no.	*Wavenumber*[(a, b)] (vac.) (cm^{-1})
1	2507·3†‡
2	2489·2$_5$†‡
3	2470·8†‡
4	2451·9†‡
5	2432·6†‡
6	2412·9†‡
7	2392·8†‡

Resolution tests: Line no. 7 unresolved doublet spacing is 0·33 cm^{-1}
Line no. 1 unresolved doublet spacing is 0·36 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 16A*).

(a) These lines are blends of two components from $H^{79}Br$ and $H^{81}Br$. Where the doublet is resolved the data from *Table 8* of Part I should be used.

(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

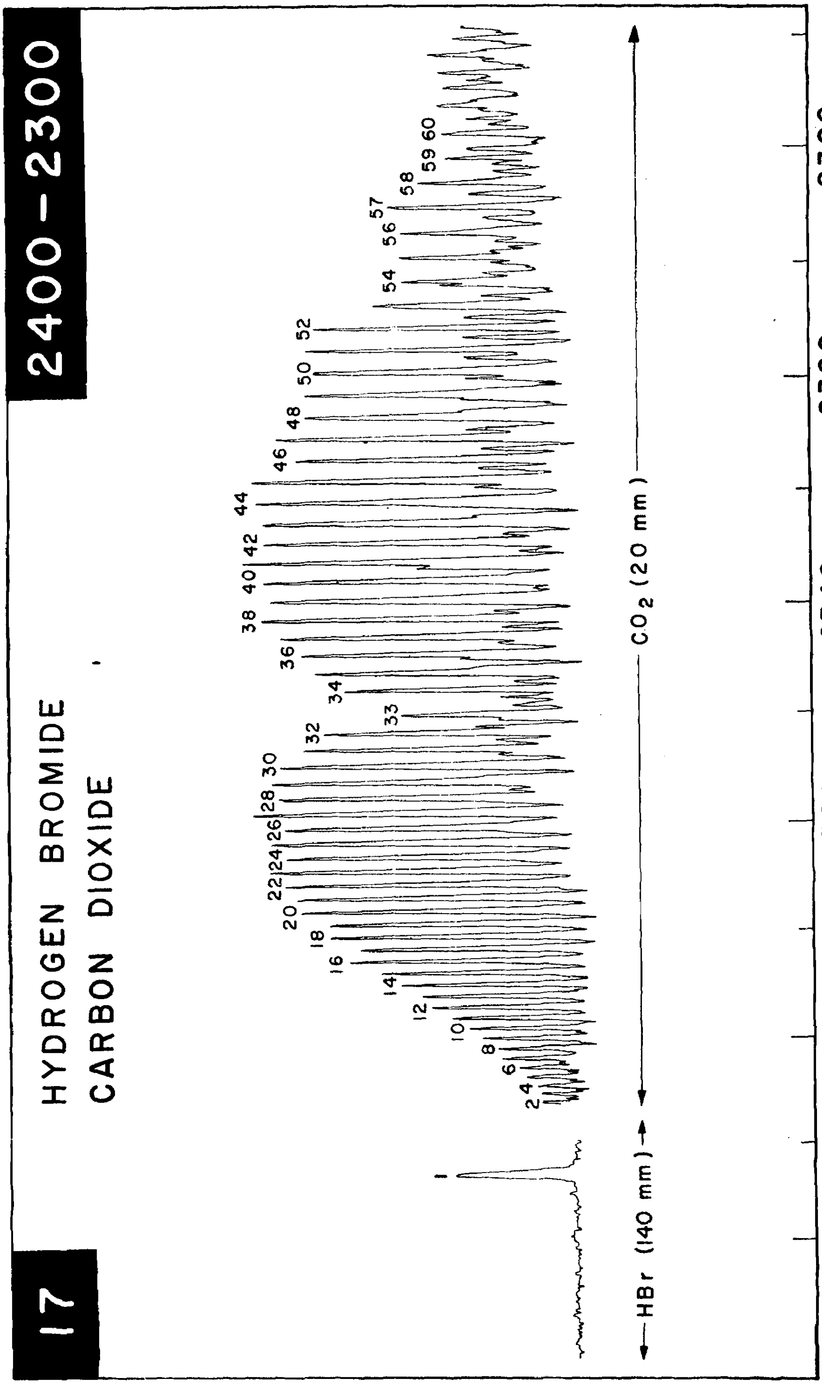

17
2400-2300
HYDROGEN BROMIDE
CARBON DIOXIDE
HBr (140 mm)
CO₂ (20 mm)
2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 33 34 36 38 40 42 44 46 48 50 52 54 56 57 58 59 60
2400
2380
2360
2340
2320
2300
WAVENUMBER (cm⁻¹)

Chart 17. Hydrogen bromide (140 mm) and carbon dioxide (20 mm): 2400–2300 cm^{-1}

Hydrogen bromide (140 mm)		*Carbon dioxide* (20 mm)					
Line no.	*Wavenumber*$^{(a,b)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})
1	2392·8†‡	2	2385·8 (±0·2 cm^{-1})	22	2365·4†	42	2334·2†‡
		3	2385·0 (±0·2 cm^{-1})	23	2364·1$_5$†	43	2332·4†‡
		4	2384·2 (±0·2 cm^{-1})	24	2362·8$_5$†	44	2330·6†‡
		5	2383·4 (±0·2 cm^{-1})	25	2361·5†	45	2328·7$_5$†‡
		6	2382·5 (±0·2 cm^{-1})	26	2360·1$_5$†	46	2326·9†‡
		7	2381·6$_5$ (±0·2 cm^{-1})	27	2358·7$_5$†	47	2325·0†‡
		8	2380·7$_5$†	28	2357·3$_5$†	48	2323·1†‡
		9	2379·8†	29	2355·9$_5$†	49	2321·1$_5$†‡
		10	2378·8$_5$†	30	2354·5†	50	2319·2†‡
		11	2377·9†	31	2353·0†	51	2317·2†‡
		12	2376·8$_5$†	32	2351·5†	52	2315·2†‡
		13	2375·8$_5$†	33	2349·9$_5$†	53	2313·2†‡
		14	2374·8†	34	2347·6†	54	2311·1†‡
		15	2373·7†	35	2346·0†	55	2309·0$_5$†‡
		16	2372·6†	36	2344·4†	56	2306·9$_5$†‡
		17	2371·4$_5$†	37	2342·7$_5$†	57	2304·8$_5$†‡
		18	2370·3†	38	2341·1†	58	2302·7†‡
		19	2369·1†	39	2339·4†‡	59	2300·5
		20	2367·9†	40	2337·7†	60	2298·3‡
		21	2366·7†	41	2335·9$_5$†		

Resolution tests: Line no. 10–line no. 11: 0·95 cm^{-1}
Line no. 48–line no. 49: 1·95 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 17A*). The weak hydrogen bromide line at 2372·3 cm^{-1} can be used as an additional calibration point.

(a) See footnote (a) to *Chart 15.*

(b) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

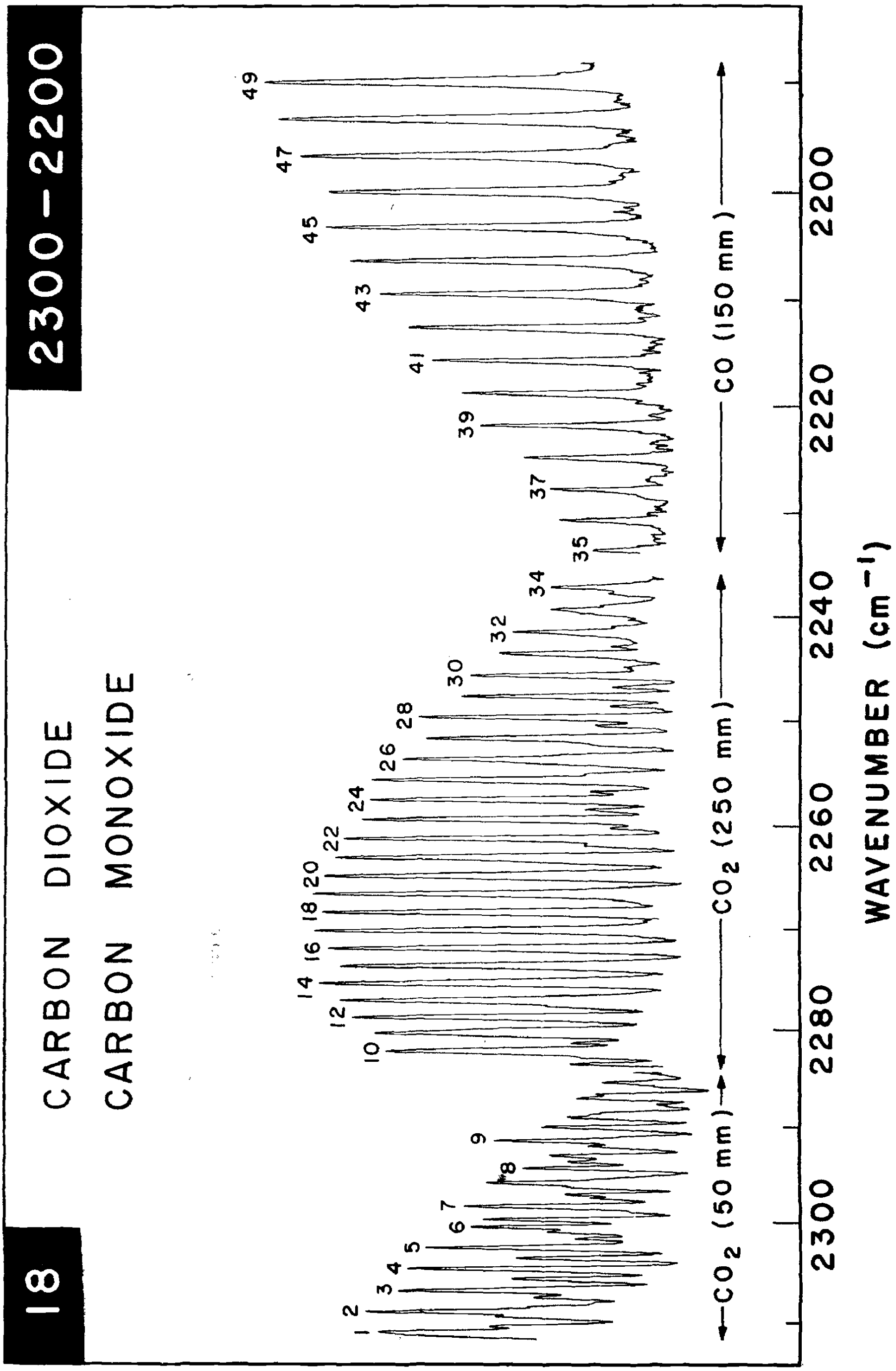

18
2300 – 2200
CARBON DIOXIDE
CARBON MONOXIDE
1
2
3
4
5
6
7
8
9
10
12
14
16
18
20
22
24
26
28
30
32
34
35
37
39
41
43
45
47
49
CO₂ (50 mm)
CO₂ (250 mm)
CO (150 mm)
2300
2280
2260
2240
2220
2200
WAVENUMBER (cm⁻¹)

Chart 18. Carbon dioxide (50 mm), carbon dioxide (250 mm) and carbon monoxide (150 mm): 2300–2200 cm^{-1}

Carbon dioxide (50 mm)		*Carbon dioxide* (250 mm)		*Carbon monoxide* (150 mm)	
Line no.	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})
1	2311·1†‡	10	2281·9$_5$†‡	35	2233·3$_5$†
		11	2280·3$_5$†	36	2230·5$_5$†
2	2309·0$_5$†‡	12	2278·7†	37	2227·6$_5$†‡
		13	2277·1†	38	2224·7†‡
3	2306·9$_5$†‡	14	2275·4†‡	39	2221·7$_5$†‡
		15	2273·7$_5$†‡	40	2218·7$_5$†‡
4	2304·8$_5$†‡	16	2272·0$_5$†‡	41	2215·7†‡
		17	2270·3†‡	42	2212·6†‡
5	2302·7†‡	18	2268·5$_5$†‡	43	2209·5†‡
		19	2266·7$_5$†‡	44	2206·3$_5$†‡
6	2300·5†‡	20	2264·9$_5$†‡	45	2203·1$_5$†‡
		21	2263·1$_5$†‡	46	2199·9$_5$†‡
7	2298·3‡ (±0·2 cm^{-1})	22	2261·3†‡	47	2196·6$_5$†‡
		23	2259·4†‡	48	2193·3$_5$†‡
8	2294·4$_5$†	24	2257·5†‡	49	2190·0†‡
		25	2255·6†‡		
9	2291·6†	26	2253·6$_5$†‡		
		27	2251·7†‡		
		28	2249·7†‡		
		29	2247·7†‡		
		30	2245·6‡		
		31	2243·5$_5$‡		
		32	2241·4$_5$‡		
		33	2239·4‡		
		34	2237·2$_5$‡		

Resolution tests: Line no. 16–line no. 17: 1·75 cm^{-1}
Line no. 46–line no. 47: 3·3 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 18A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

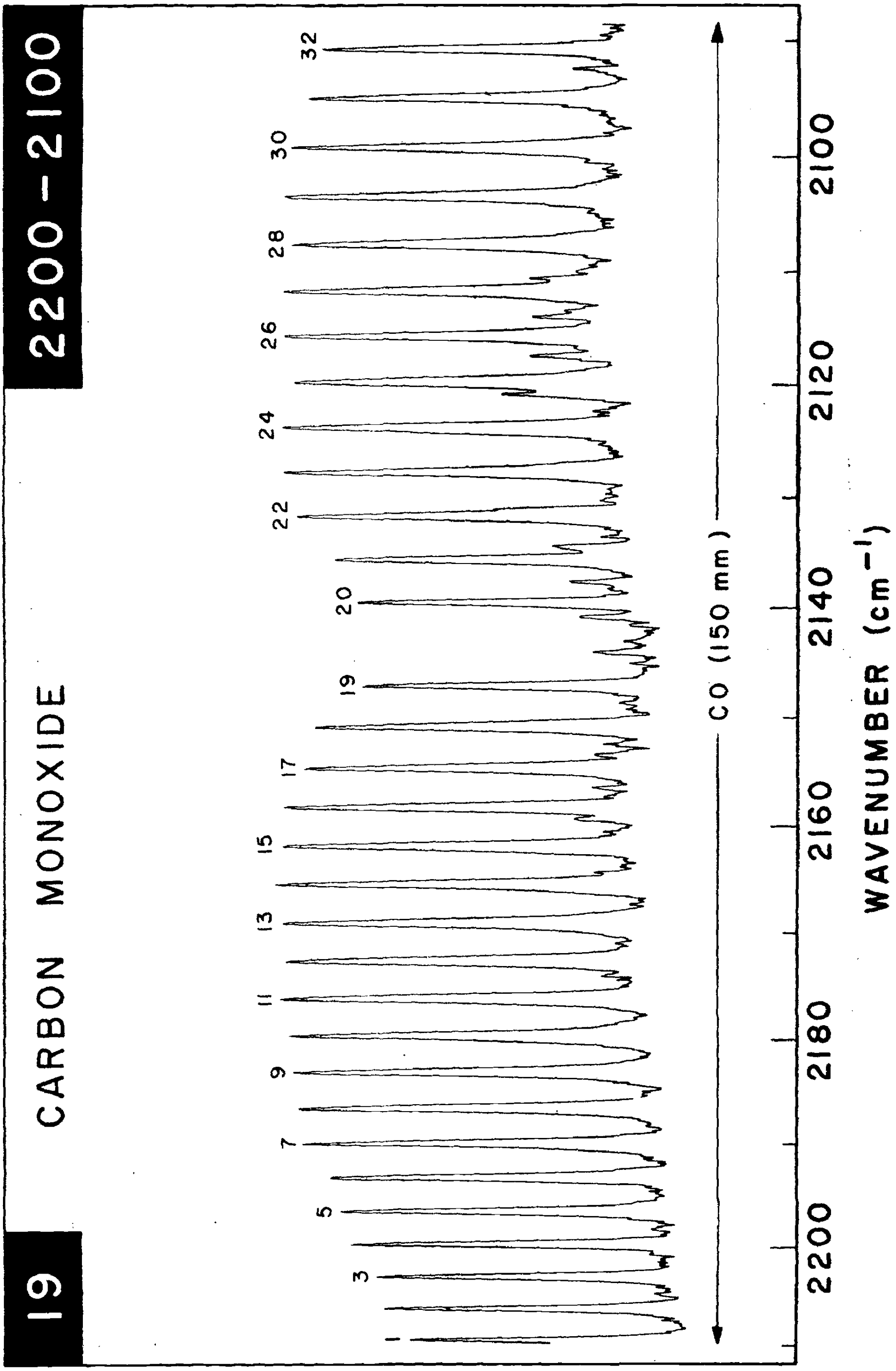

19
CARBON MONOXIDE
2200 - 2100
3
5
7
9
11
13
15
17
19
20
22
24
26
28
30
32
CO (150 mm)
2200
2180
2160
2140
2120
2100
WAVENUMBER (cm⁻¹)

Chart 19. Carbon monoxide (150 mm): 2200–2100 cm^{-1}

Line no.	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})
1	2209·5†‡	17	2154·6†‡
2	2206·3$_5$†‡	18	2150·8$_5$†‡
3	2203·1$_5$†‡	19	2147·1†‡
4	2199·9$_5$†‡	20	2139·4$_5$†‡
5	2196·6$_5$†‡	21	2135·5$_5$†‡
6	2193·3$_5$†‡	22	2131·6$_5$†‡
7	2190·0†‡	23	2127·7†‡
8	2186·6$_5$†‡	24	2123·7†‡
9	2183·2$_5$†‡	25	2119·7†‡
10	2179·7$_5$†‡	26	2115·6$_5$†‡
11	2176·3†‡	27	2111·5$_5$†‡
12	2172·7$_5$†‡	28	2107·4†‡
13	2169·2†‡	29	2103·2$_5$†‡
14	2165·6†‡	30	2099·1†‡
15	2161·9$_5$†‡	31	2094·8$_5$†‡
16	2158·3†‡	32	2090·6†‡

Resolution tests: Line no. 7–line no. 8: 3·35 cm^{-1}
Line no. 30–line no. 31: 4·25 cm^{-1}

---

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 19A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

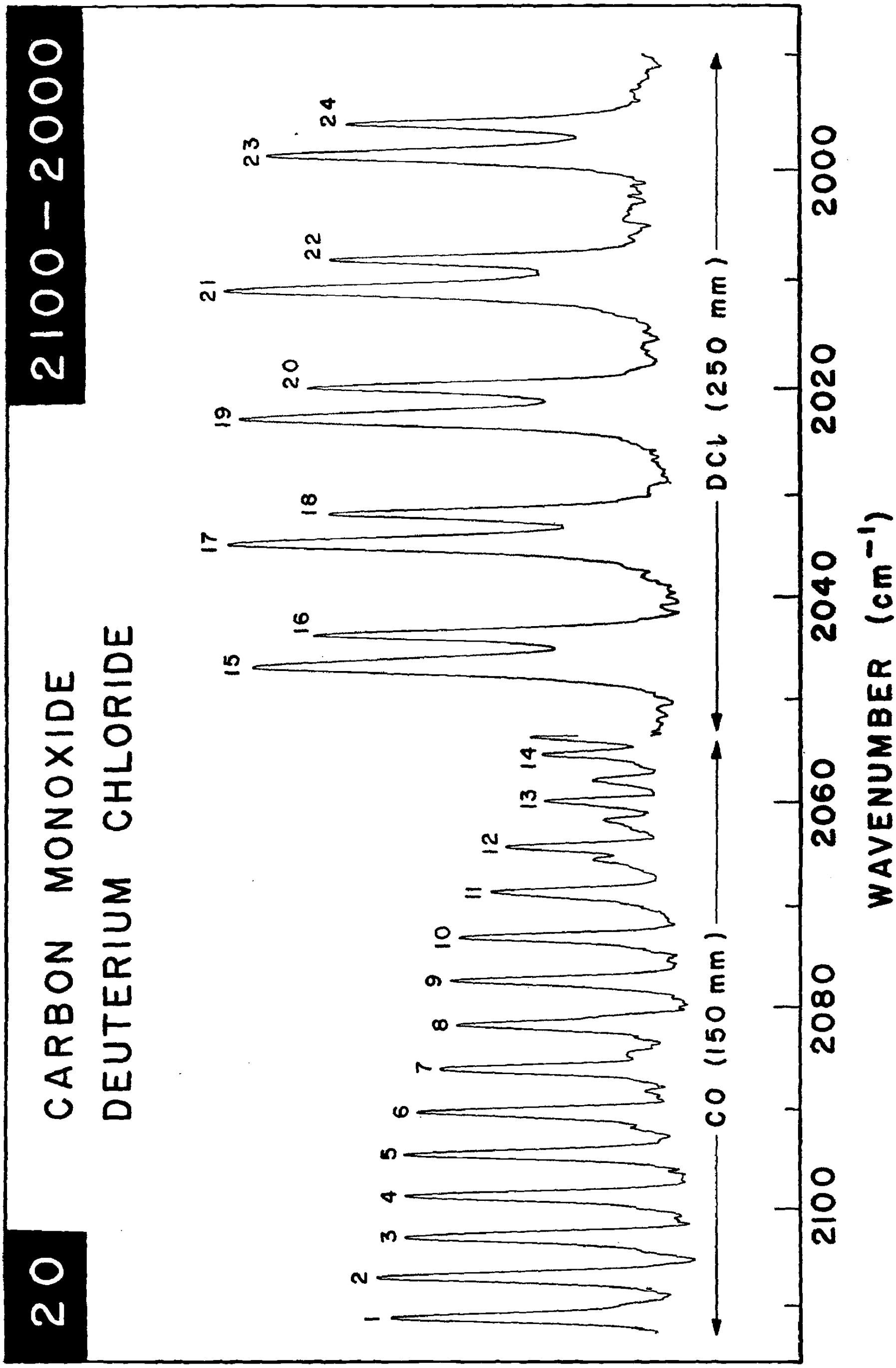

20
2100 – 2000
CARBON MONOXIDE
DEUTERIUM CHLORIDE
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
CO (150 mm)
DCl (250 mm)
2100
2080
2060
2040
2020
2000
WAVENUMBER (cm⁻¹)

Chart 20. Carbon monoxide (150 mm) and deuterium chloride (250 mm): 2100–2000 cm^{-1}

Carbon monoxide (150 mm) *Line no.*	Wavenumber[(a)] (vac.) (cm^{-1})	*Deuterium chloride* (250 mm) *Line no.*	*Wavenumber*[(a, b)] (vac.) (cm^{-1})		
1	2111·5$_5$†‡	15	2046·6†	(2045·9)	(±0·3 cm^{-1})
2	2107·4†‡	16	2043·7$_5$†		
3	2103·2$_5$†‡	17	2034·9$_5$†	(2034·2$_5$)	(±0·3 cm^{-1})
4	2099·1†‡	18	2032·1†		
5	2094·8$_5$†‡	19	2023·1†‡	(2022·4)	(±0·3 cm^{-1})
6	2090·6†‡	20	2020·3†		
7	2086·3†‡	21	2011·0$_5$†‡	(2010·3$_5$)	(±0·3 cm^{-1})
8	2082·0†‡	22	2008·2$_5$†		
9	2077·6$_5$†‡	23	1998·7$_5$†‡	(1998·1)	(±0·3 cm^{-1})
10	2073·2$_5$†‡	24	1996·0$_5$†		
11	2068·8$_5$†‡				
12	2064·4†‡				
13	2059·9†				
14	2055·4†				

Resolution tests: Line no. 23–line no. 24: 2·7 cm^{-1}
Line no. 2–line no. 3: 4·15 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 20A*).

(a) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

(b) Under lower resolution the position of the more intense (D^{35}Cl) peak of each doublet is not significantly displaced provided the two peaks are separately resolved, as shown in *Charts 20A* and *21A*. If the resolution is further diminished, so that the lines blend, the main peak is displaced to lower wavenumber. If the blended line appears symmetrical, the position of the peak corresponds approximately to the weighted average of the positions of the two component lines, based on the ^{35}Cl/^{37}Cl abundance ratio of 0·75. These values are given in parentheses in the tables accompanying *Charts 20* and *21*.

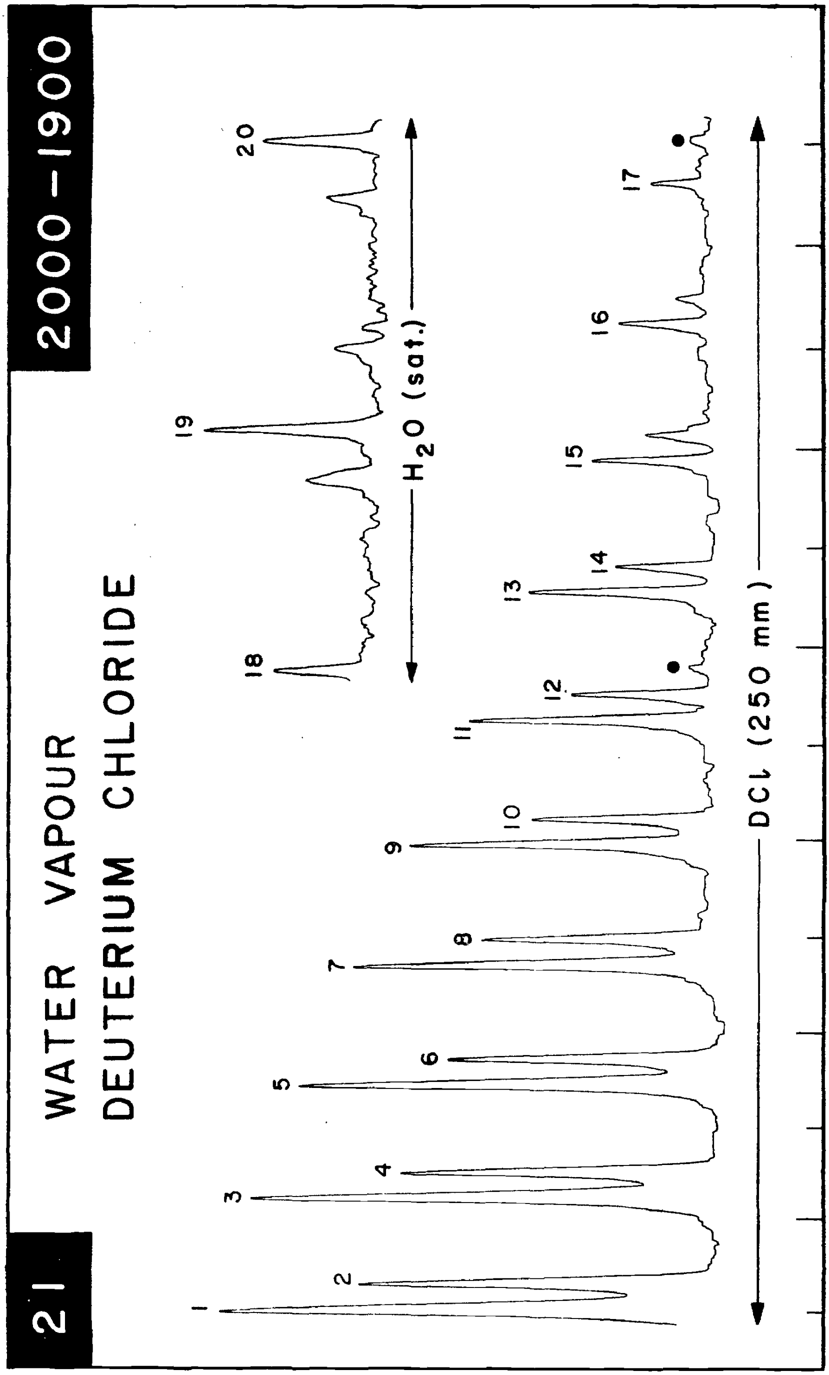

21
2000 – 1900
WATER VAPOUR
DEUTERIUM CHLORIDE
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
H_2O (sat.)
DCl (250 mm)
2000
1980
1960
1940
1920
1900
WAVENUMBER (cm^{-1})

Chart 21. Deuterium chloride (250 mm) and water vapour (saturated): 2000–1900 cm^{-1}

Deuterium chloride (250 mm)				*Water vapour (saturated)*	
Line no.	*Wavenumber*$^{(a,b,c)}$ (vac.) (cm^{-1})			*Line no.*	*Wavenumber*$^{(c)}$ (vac.) (cm^{-1})
1	2011·0$_5$†‡	(2010·3$_5$)	(±0·3 cm^{-1})	18	1942·6‡
2	2008·2$_5$†				
3	1998·7$_5$†‡	(1998·1)	(±0·3 cm^{-1})	19	1918·0$_5$‡
4	1996·0$_5$†				
5	1986·3†‡	(1985·6$_5$)	(±0·3 cm^{-1})	20	1889·6†‡
6	1983·6$_5$†				
7	1973·6$_5$†‡	(1973·0)	(±0·3 cm^{-1})		
8	1971·0†				
9	1960·8†‡	(1960·1$_5$)	(±0·3 cm^{-1})		
10	1958·2†				
11	1947·7$_5$†‡	(1947·1$_5$)	(±0·3 cm^{-1})		
12	1945·2†				
13	1934·5$_5$†‡	(1933·9$_5$)	(±0·3 cm^{-1})		
14	1932·0$_5$†				
15	1921·1$_5$†‡	(1920·5$_5$)	(±0·3 cm^{-1})		
16	1907·6†‡	(1907·0)	(±0·3 cm^{-1})		
17	1893·8$_5$‡		(±0·2 cm^{-1})		

Resolution tests: Line no. 13–line no. 14: 2·5 cm^{-1}
Line no. 1–line no. 2: 2·8 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 21A*). See also footnote (a) to *Chart 20.*

(a) See footnote (a) to *Chart 20.*

(b) Black circles indicate positions of prominent atmospheric water vapour lines.

(c) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

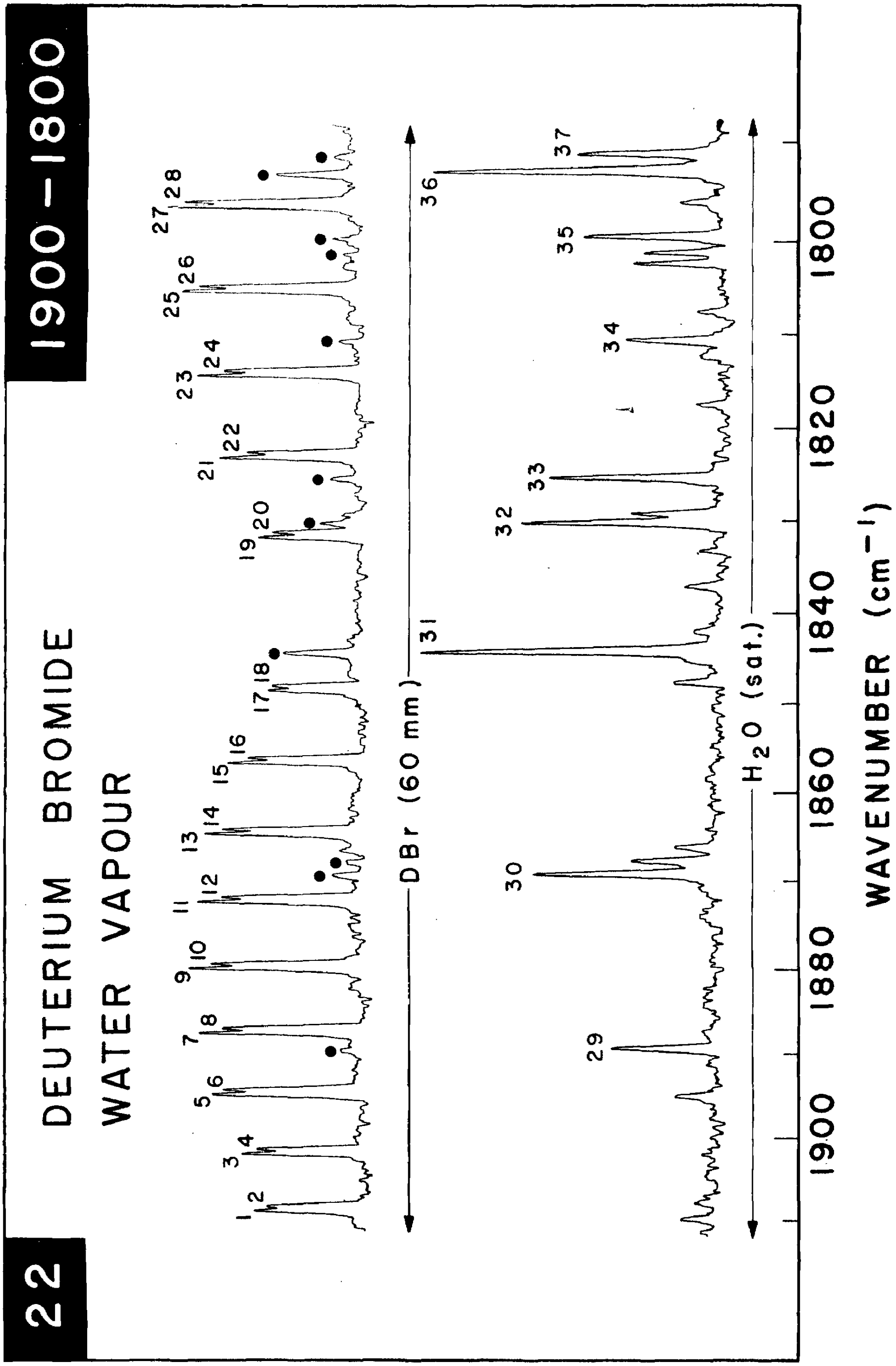

22
1900–1800
DEUTERIUM BROMIDE
WATER VAPOUR
DBr (60 mm)
H_2O (sat.)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
1900
1880
1860
1840
1820
1800
WAVENUMBER (cm⁻¹)

Chart 22. Deuterium bromide (60 mm) and water vapour (saturated): 1900–1800 cm^{-1}

	Deuterium bromide (60 mm)					*Water vapour* (*saturated*)	
Line no.	*Wavenumber*$^{(a, b)}$ (vac.) (cm^{-1})		*Line no.*	*Wavenumber*$^{(a, b)}$ (vac.) (cm^{-1})		*Line no.*	*Wavenumber*$^{(d)}$ (vac.) (cm^{-1})
1	1908·7$_5$†	(1908·4$_5$)	15	1856·5$_5$†	(1856·2$_5$)	29	1889·6†‡
2	1908·1†		16	1856·0†		30	1869·3$_5$†
3	1901·8$_5$†	(1901·5$_5$)	17	1848·4†	(1848·1$_5$)	31	1844·2$_5$‡$^{(c)}$
4	1901·2$_5$†		18	1847·9†		32	1830·2$_5$‡
5	1894·7$_5$†	(1894·4$_5$)	19	1831·5$_5$†	(1831·3)	33	1825·2$_5$†
6	1894·1$_5$†		20	1831·0$_5$†		34	1810·6$_5$†
7	1887·4$_5$†	(1887·1$_5$)	21	1822·9†	(1822·6$_5$)	35	1799·6†
8	1886·9†		22	1822·4†		36	1792·6$_5$‡
9	1880·0†	(1879·7$_5$)	23	1814·1†	(1813·8$_5$)	37	1790·9$_5$
10	1879·5†		24	1813·6†			
11	1872·3$_5$†	(1872·1)	25	1805·1†	(1804·8$_5$)		
12	1871·8†		26	1804·6†			
13	1864·5$_5$†	(1864·2$_5$)	27	1795·9$_5$†	(1795·7$_5$)		
14	1864·0†		28	1795·5†			

Resolution tests:
Line no. 27–line no. 28: 0·45 cm^{-1}
Line no. 1–line no. 2: 0·65 cm^{-1}
Line no. 36–line no. 37: 1·7 cm^{-1}

---

† Part I calibration lines.
‡ Suitable for use under lower resolution (*Chart 22A*), see also footnote (a) below.
(a) Where the D^{79}Br and D^{81}Br doublet is not resolved a mean value for the peak positions may be used (these figures are given in parentheses).
(b) Black circles indicate positions of prominent atmospheric water vapour lines.
(c) Blend of two component lines.
(d) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

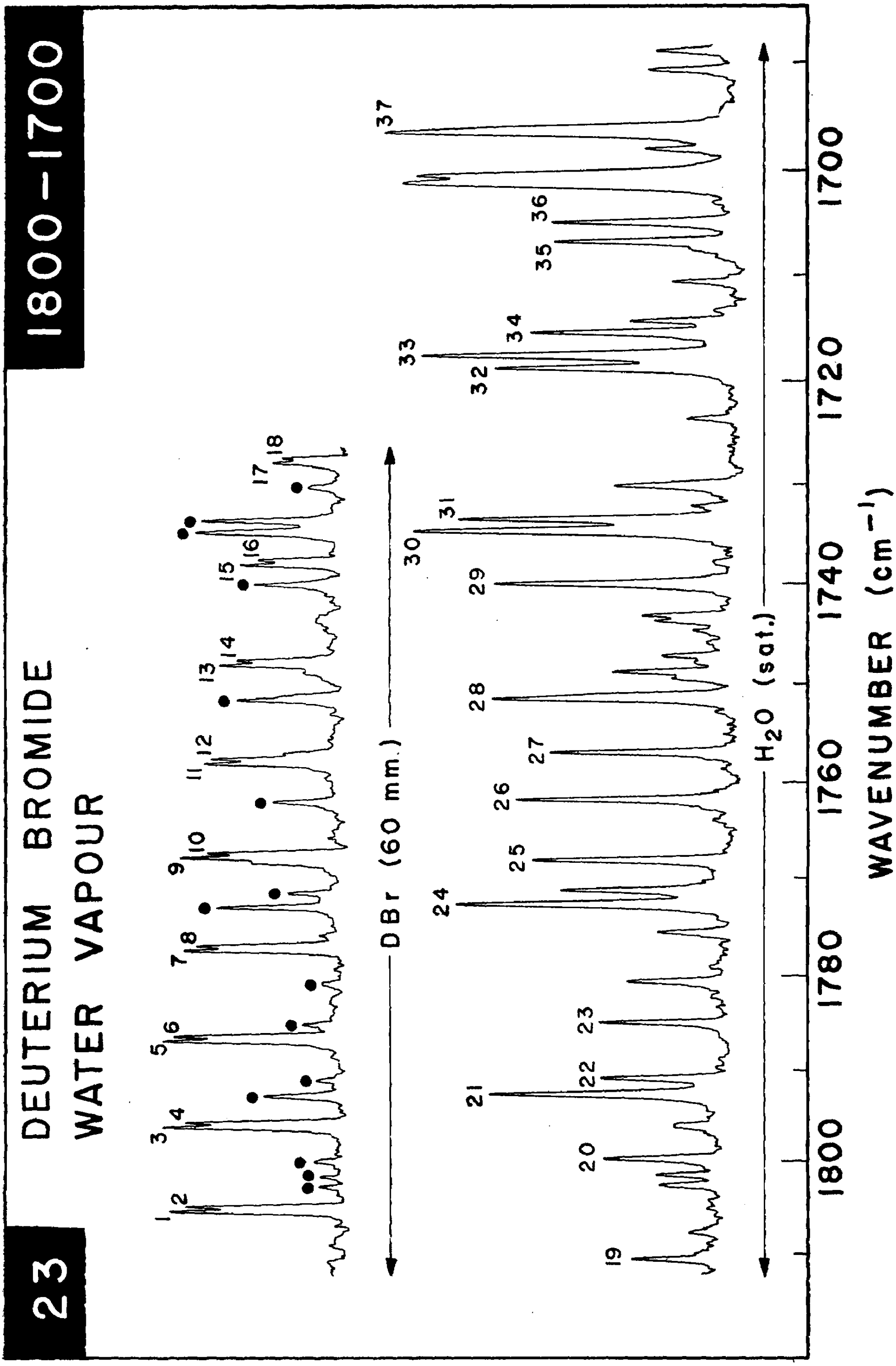

23
1800–1700
DEUTERIUM BROMIDE
WATER VAPOUR
DBr (60 mm.)
H₂O (sat.)
WAVENUMBER (cm⁻¹)
1800
1780
1760
1740
1720
1700
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37

Chart 23. Deuterium bromide (60 mm) and water vapour (saturated): 1800–1700 cm^{-1}

Deuterium bromide (60 mm)			*Water vapour* (*saturated*)	
Line no.	*Wavenumber*$^{(a,b)}$ (vac.) (cm^{-1})		*Line no.*	*Wavenumber*$^{(c)}$ (vac.) (cm^{-1})
1	1805·1†	(1804·8$_5$)	19	1810·6$_5$†
2	1804·6†		20	1799·6†
3	1795·9$_5$†	(1795·7$_5$)	21	1792·6$_5$‡
4	1795·5†		22	1790·9$_5$
5	1786·6$_5$†	(1786·4)	23	1784·9$_5$†‡
6	1786·2†		24	1772·6$_5$
7	1777·2†	(1776·9$_5$)	25	1768·1$_5$†
8	1776·7†		26	1761·9‡
9	1767·6†	(1767·3$_5$)	27	1756·8†‡
10	1767·1†		28	1751·4$_5$
11	1757·8$_5$†	(1757·6)	29	1739·8$_5$‡
12	1757·4†		30	1734·6$_5$
13	1747·9$_5$†	(1747·7)	31	1733·4$_5$
14	1747·4$_5$†		32	1718·6$_5$
15	1737·9†	(1737·6$_5$)	33	1717·4$_5$‡
16	1737·4$_5$†		34	1715·2
17	1727·7†	(1727·5)	35	1706·3$_5$
18	1727·2$_5$†		36	1704·5
			37	1695·9$_5$‡

Resolution tests:
Line no. 11–line no. 12: 0·45 cm^{-1}
Line no. 30–line no. 31: 1·2 cm^{-1}
Line no. 21–line no. 22: 1·7 cm^{-1}

---

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 23A*), see also footnote (a) below.

(a) Where the D^{79}Br and D^{81}Br doublet is not resolved, a mean value for the peak positions may be used (these figures are given in parentheses).

(b) Black circles indicate positions of prominent atmospheric water vapour lines.

(c) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

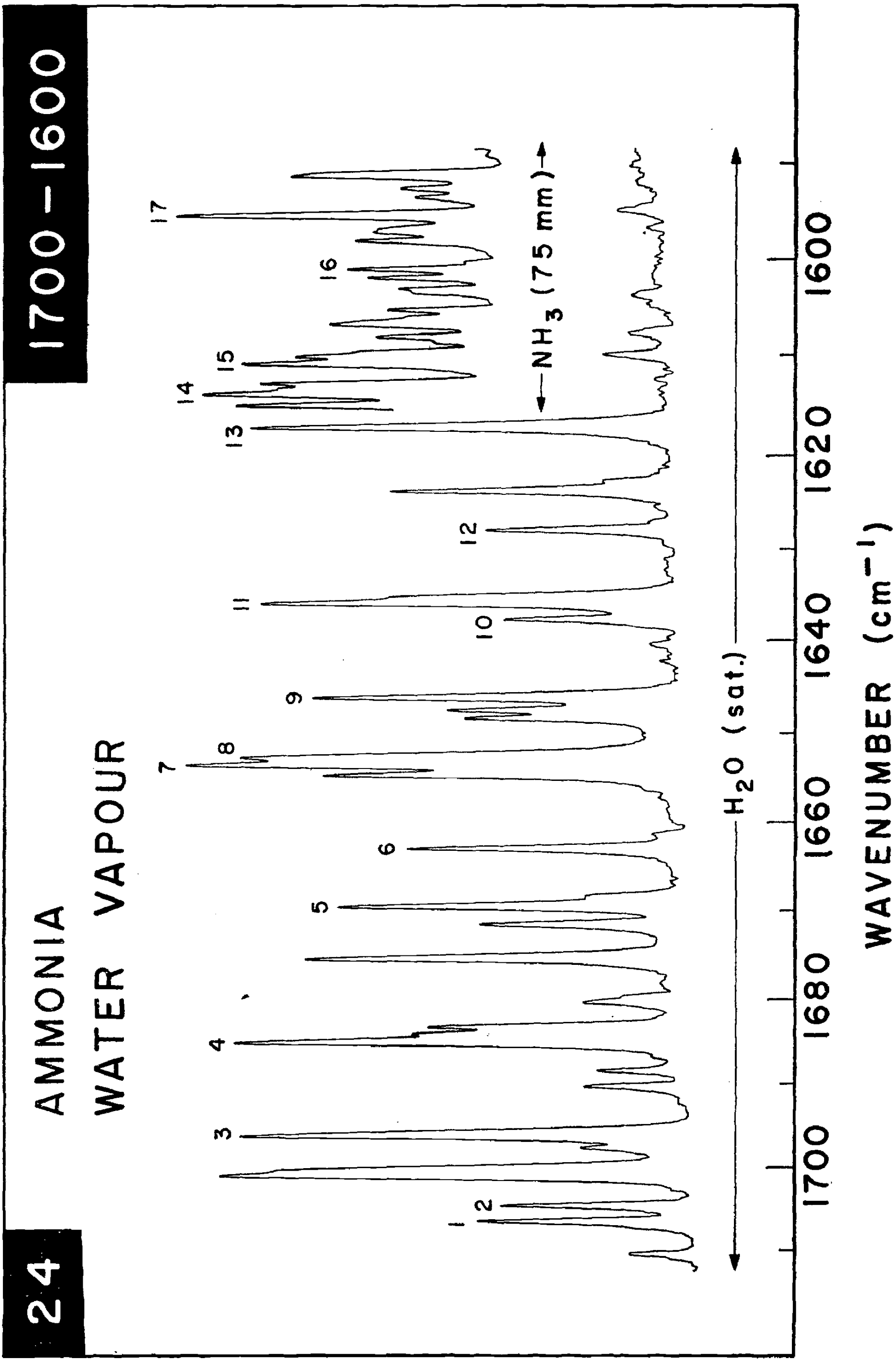

24
1700 – 1600
AMMONIA
WATER VAPOUR
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
H₂O (sat.)
NH₃ (75 mm)
1700
1680
1660
1640
1620
1600
WAVENUMBER (cm⁻¹)

Chart 24. Water vapour (saturated) and ammonia (75 mm): 1700–1600 cm^{-1}

Water vapour (saturated)		*Ammonia*(75 mm)	
Line no.	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})
1	1706·3$_5$	14	1613·3$_5$ (±0·2 cm^{-1})
2	1704·5	15	1610·3$_5$ (±0·2 cm^{-1})
3	1695·9$_5$‡	16	1600·6 (±0·2 cm^{-1})
4	1684·9	17	1594·8$_5$‡ (±0·2 cm^{-1})
5	1669·4$_5$‡		
6	1662·8†‡		
7	1653·3$_5$‡		
8	1652·4$_5$		
9	1646·0		
10	1637·5$_5$†		
11	1635·6‡		
12	1627·8†		
13	1616·7†‡		

Resolution tests: Line no. 7–line no. 8: 0·9 cm^{-1}
Line no. 1–line no. 2: 1·85 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 24A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.

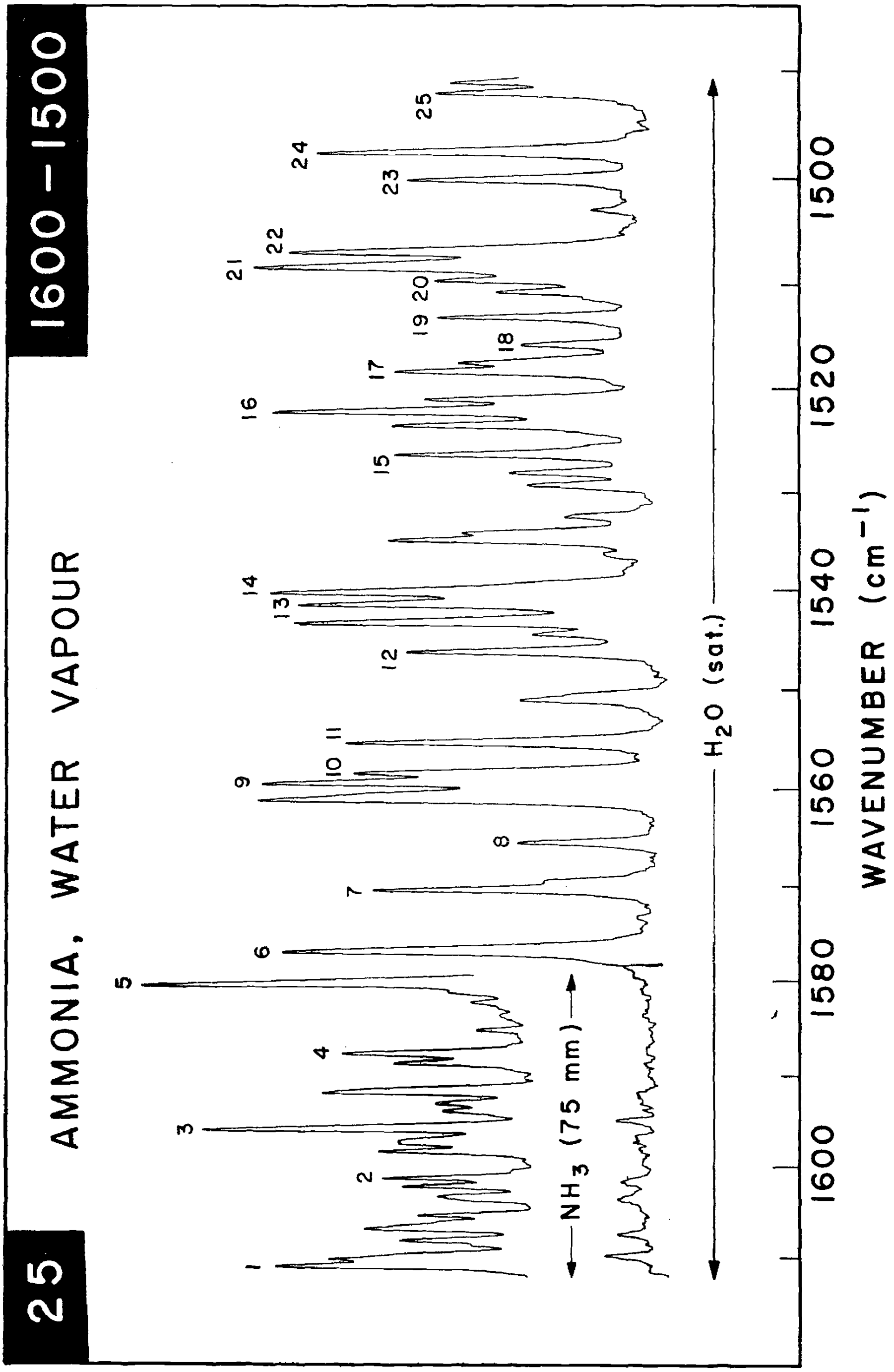

25
1600 – 1500
AMMONIA, WATER VAPOUR
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
NH_3 (75 mm)
H_2O (sat.)
1600
1580
1560
1540
1520
1500
WAVENUMBER (cm^{-1})

Chart 25. Ammonia (75 mm) and water vapour (saturated): 1600–1500 cm^{-1}

Ammonia (75 mm)		*Water vapour* (*saturated*)			
Line no.	*Wavenumber* (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})
1	1610·3$_5$ (±0·2 cm^{-1})	6	1576·2†‡	17	1517·5
2	1600·6 (±0·2 cm^{-1})	7	1569·8$_5$	18	1515·0
3	1594·8$_5$ (±0·2 cm^{-1})	8	1564·8$_5$†‡	19	1512·3†
4	1586·9 (±0·2 cm^{-1})	9	1558·5$_5$	20	1508·6
5	1579·5‡$^{(b)}$ (±0·2 cm^{-1})	10	1557·5$_5$	21	1507·1
		11	1554·4‡	22	1505·6$_5$
		12	1545·1$_5$†	23	1498·8$_5$†
		13	1540·3	24	1496·2$_5$‡
		14	1539·0$_5$	25	1490·8$_5$
		15	1525·5		
		16	1521·4‡		

Resolution tests:
Line no. 9–line no. 10: 1·0 cm^{-1}
Line no. 13–line no. 14: 1·25 cm^{-1}
Line no. 21–line no. 22: 1·45 cm^{-1}

---

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 25A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1} unless otherwise indicated.
(b) Blend of two component lines.

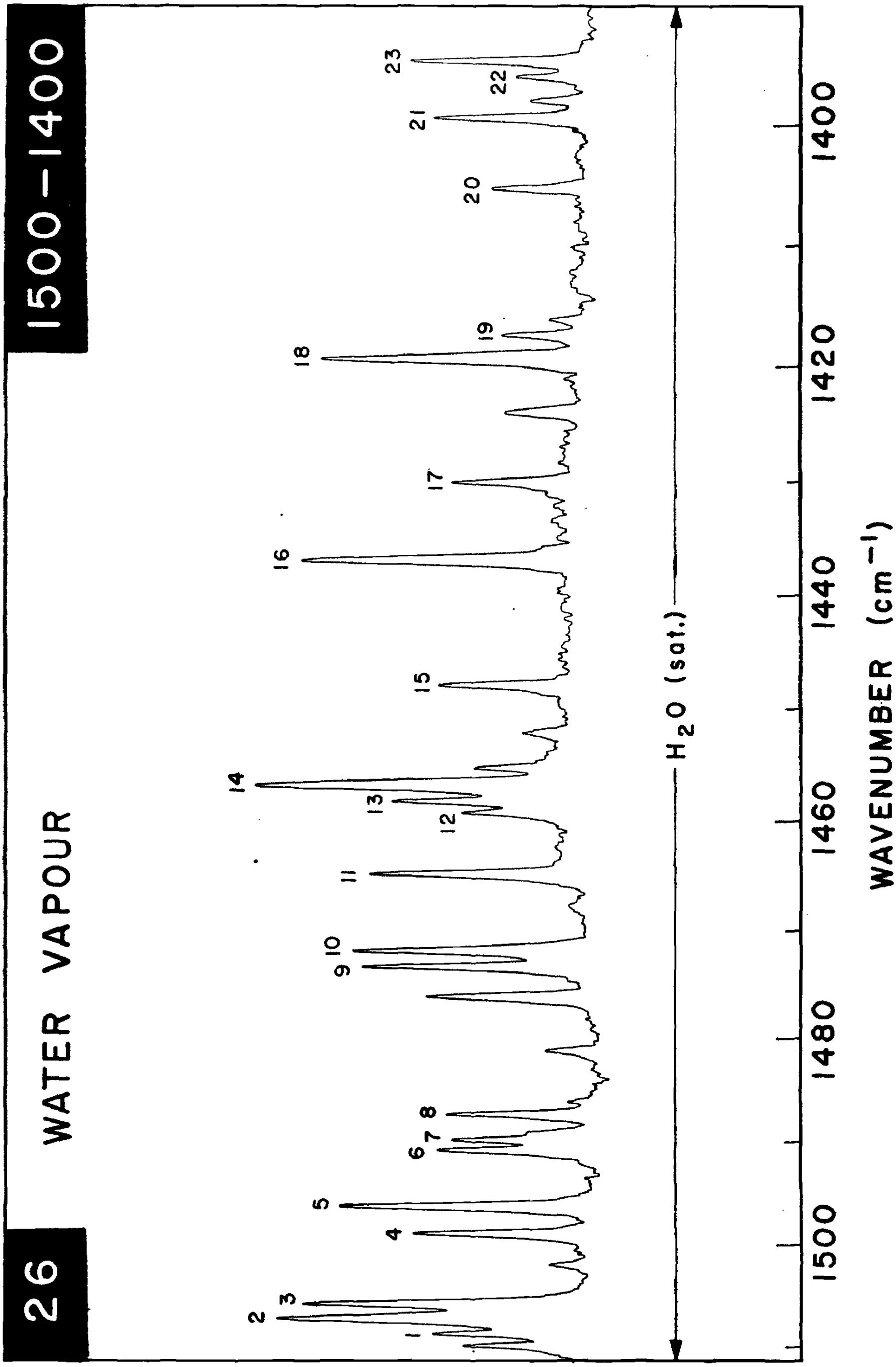

26
1500 – 1400
WATER VAPOUR
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
H$_2$O (sat.)
1500
1480
1460
1440
1420
1400
WAVENUMBER (cm^{-1})

Chart 26. Water vapour (saturated): 1500–1400 cm^{-1}

Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	1508·6	13	1458·2$_5$
2	1507·1	14	1456·8‡(b)
3	1505·6$_5$	15	1447·9$_5$†‡
4	1498·8†	16	1436·7‡
5	1496·2$_5$‡	17	1429·9$_5$†‡
6	1490·8$_5$	18	1419·3‡
7	1489·8$_5$	19	1417·4$_5$†
8	1487·3†	20	1405·0†‡
9	1473·5	21	1399·1$_5$‡
10	1472·0$_5$	22	1395·8
11	1464·9†‡	23	1394·4$_5$†
12	1459·3		

Resolution tests: Line no. 6–line no. 7: 1·0 cm^{-1}
Line no. 22–line no. 23: 1·35 cm^{-1}
Line no. 9–line no. 10: 1·45 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 26A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) Blend of two component lines.

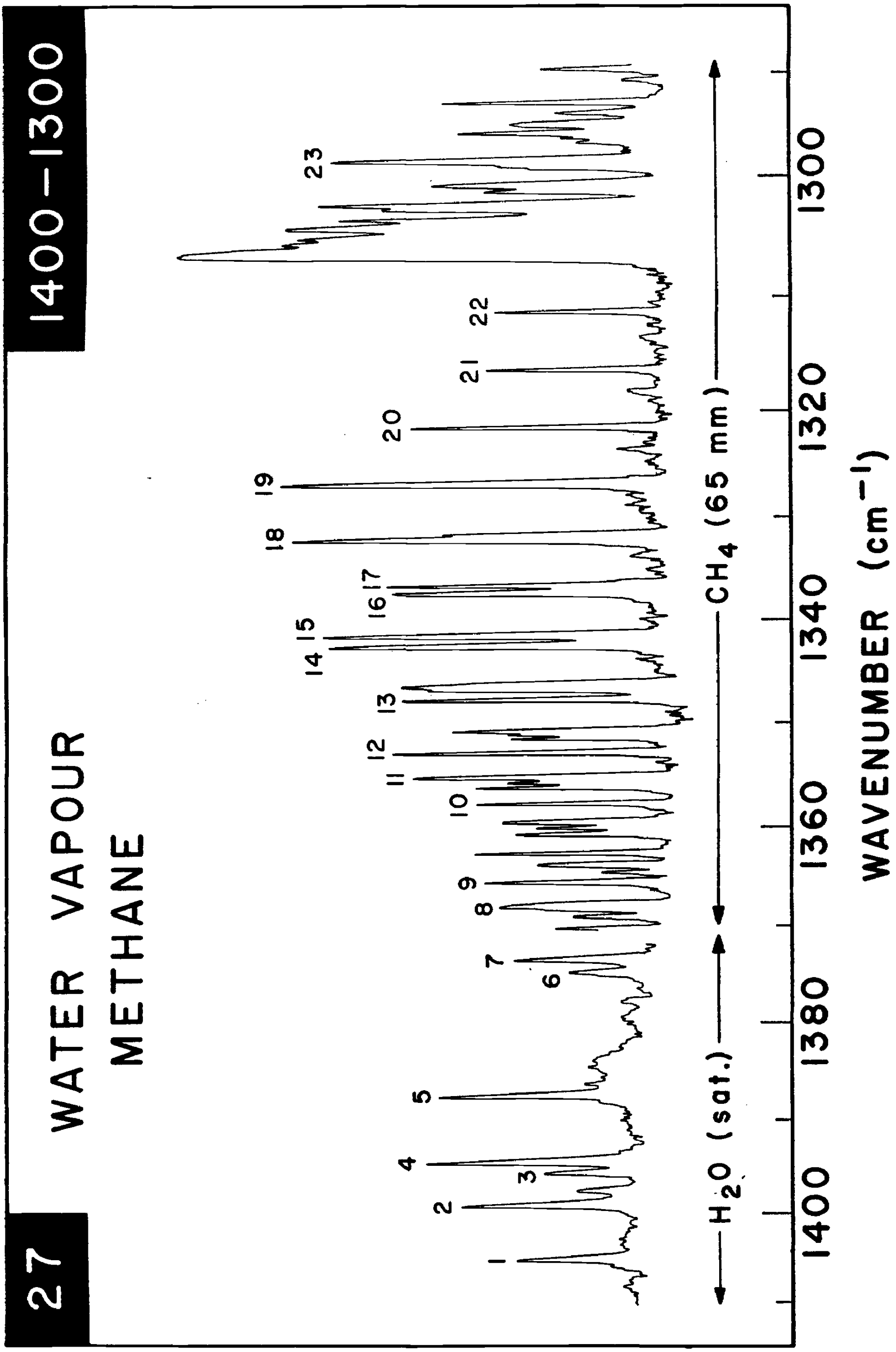

27
1400–1300
WATER VAPOUR
METHANE
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
H$_2$O (sat.)
CH$_4$ (65 mm)
1400
1380
1360
1340
1320
1300
WAVENUMBER (cm^{-1})

Chart 27. Water vapour (saturated) and methane (60 mm): 1400–1300 cm^{-1}

Water vapour (saturated)		*Methane* (60 mm)			
Line no.	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})
1	1405·0†‡	8	1368·5$_5$‡	16	1337·6$_5$
2	1399·1$_5$‡	9	1366·0$_5$†	17	1336·8$_5$
3	1395·8	10	1358·1	18	1332·4†‡
4	1394·4$_5$†	11	1355·5$_5$	19	1327·2†‡
5	1387·5$_5$	12	1353·0$_5$†	20	1322·1†‡
6	1375·1†	13	1347·9	21	1316·8‡
7	1373·7$_5$	14	1342·8	22	1311·4†‡
		15	1341·8†	23	1297·6$_5$†‡

Resolution tests: Line no. 16–line no. 17: 0·8 cm^{-1}
Line no. 14–line no. 15: 1·0 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 27A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

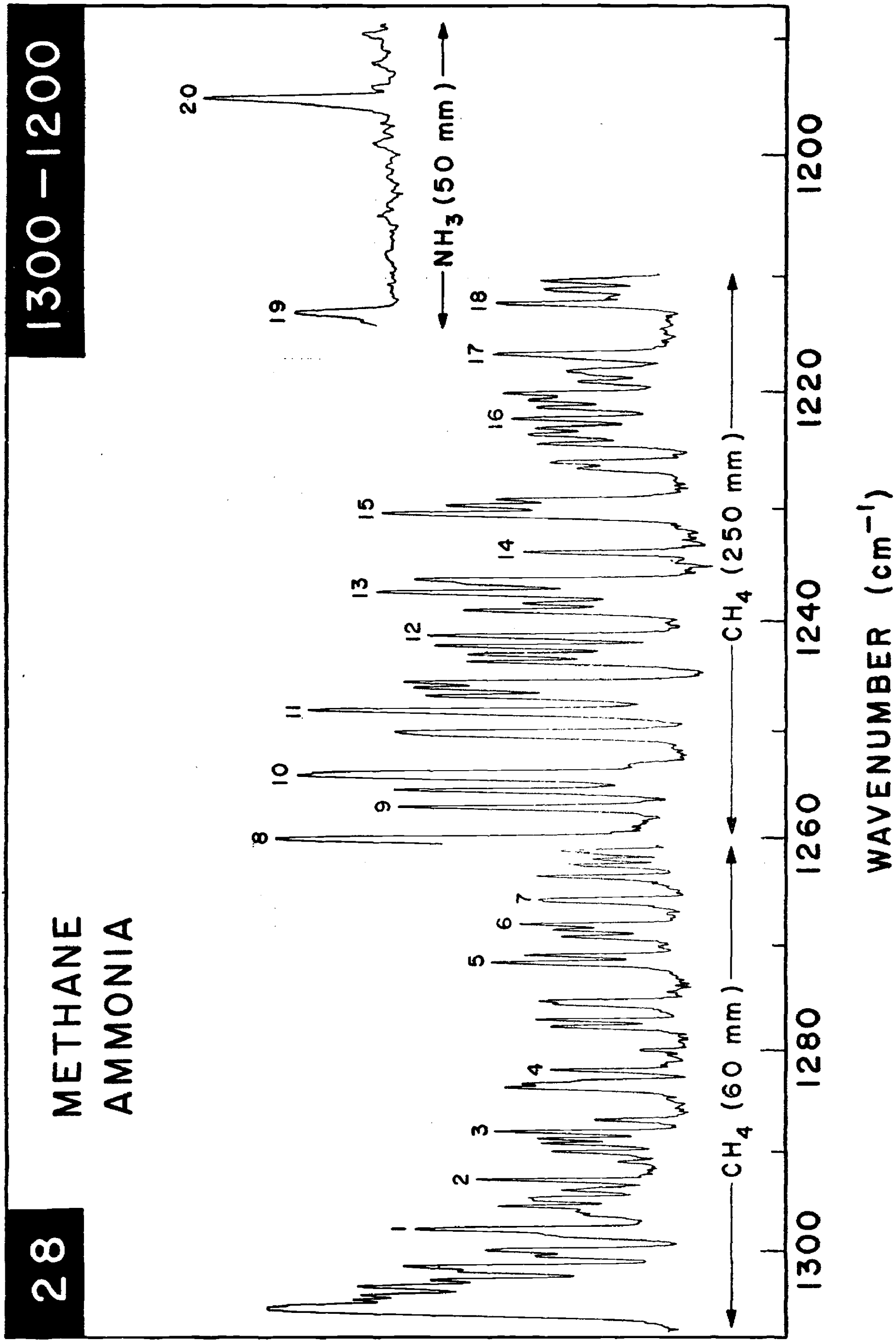

28
1300 – 1200
METHANE
AMMONIA
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
CH_4 (60 mm)
CH_4 (250 mm)
NH_3 (50 mm)
1300
1280
1260
1240
1220
1200
WAVENUMBER (cm^{-1})

Chart 28. Methane (65 mm), (250 mm) and ammonia (50 mm): 1300–1200 cm^{-1}

Methane (65 mm)		*Methane* (250 mm)		*Ammonia* (50 mm)	
Line no.	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(a)}$ (vac.) (cm^{-1})
1	$1297{\cdot}6_5$†‡	8	$1259{\cdot}7_5$	19	1212·7†‡
2	1292·6†	9	1256·6†	20	1195·0†‡
3	1287·8	10	$1253{\cdot}7_5$‡		
4	1281·6†	11	1247·8†		
5	1271·5	12	1241·0		
6	1267·9	13	1237·2‡		
7	1265·5†‡	14	$1233{\cdot}4_5$		
		15	1230·1		
		16	1221·9		
		17	$1216{\cdot}2_5$		
		18	1211·9		

† Part I calibration band.
‡ Suitable for use at lower resolution (*Chart 28A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

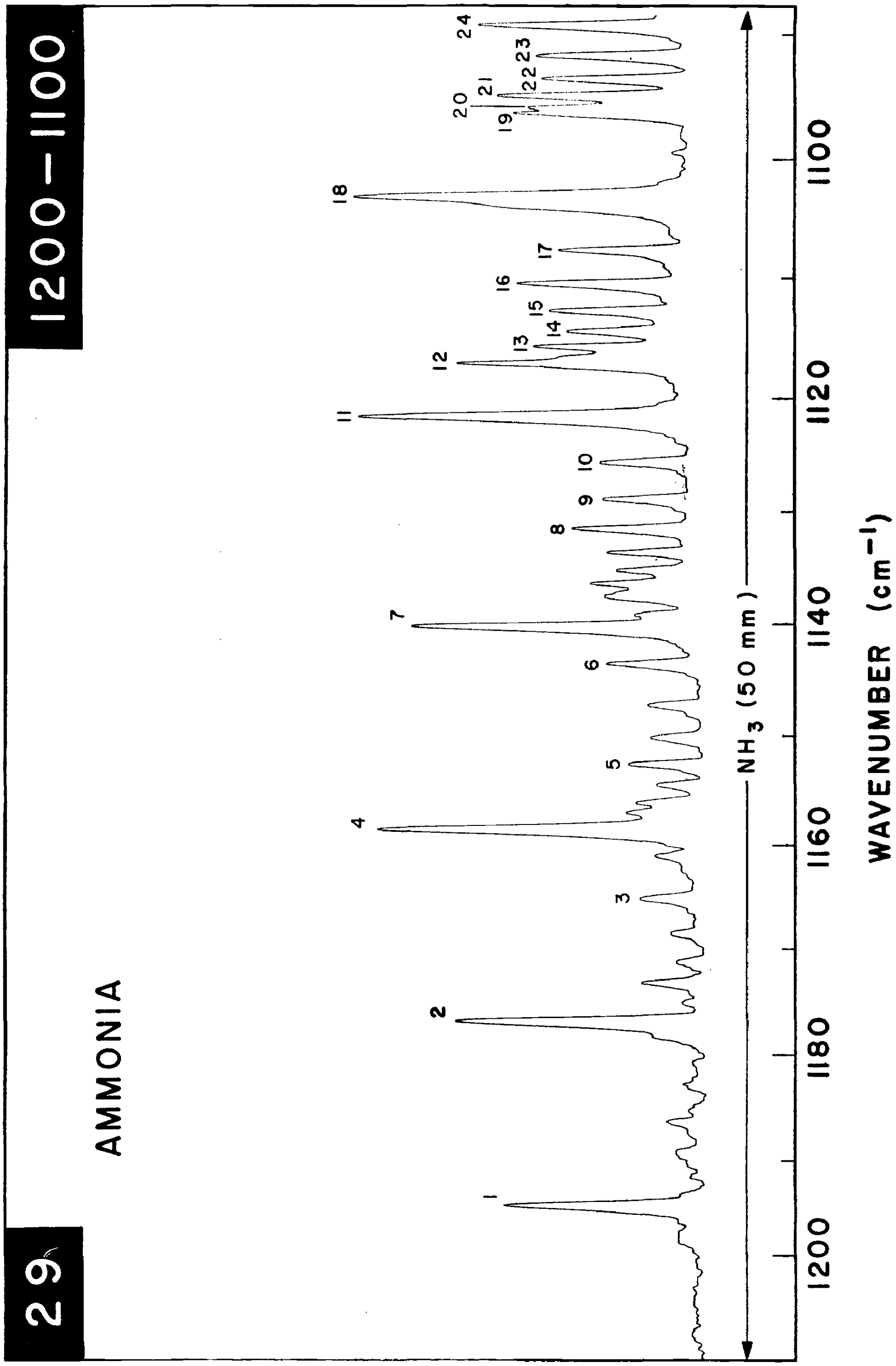

29
1200—1100
AMMONIA
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
NH$_3$ (50 mm)
1200
1180
1160
1140
1120
1100
WAVENUMBER (cm^{-1})

Chart 29. Ammonia (50 mm): 1200–1100 cm^{-1}

Line no.	*Wavenumber*[(a)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(a)] (vac.) (cm^{-1})
1	1195·0†‡	13	$1116{\cdot}0_5$†
2	1177·1†‡	14	1114·7
3	1165·5	15	$1112{\cdot}9_5$
4	$1158{\cdot}9_5$†‡	16	1110·7†
5	$1152{\cdot}8_5$†	17	$1107{\cdot}8_5$
6	1143·9†	18	$1103{\cdot}4_5$†‡
7	$1140{\cdot}6_5$†‡	19	1096·7
8	$1131{\cdot}8_5$†	20	$1096{\cdot}1_5$
9	$1129{\cdot}2_5$	21	$1095{\cdot}1_5$†
10	$1126{\cdot}0_5$†	22	$1093{\cdot}7_5$
11	$1122{\cdot}1_5$†‡	23	$1091{\cdot}8_5$
12	$1117{\cdot}5_5$		

Resolution tests: Line no. 19–line no. 20: 0·55 cm^{-1}
Line no. 12–line no. 13: 1·5 cm^{-1}
Line no. 8–line no. 9: 2·6 cm^{-1}

† Part I calibration line.

‡ Suitable for use under lower resolution (*Chart 29A*).

(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.

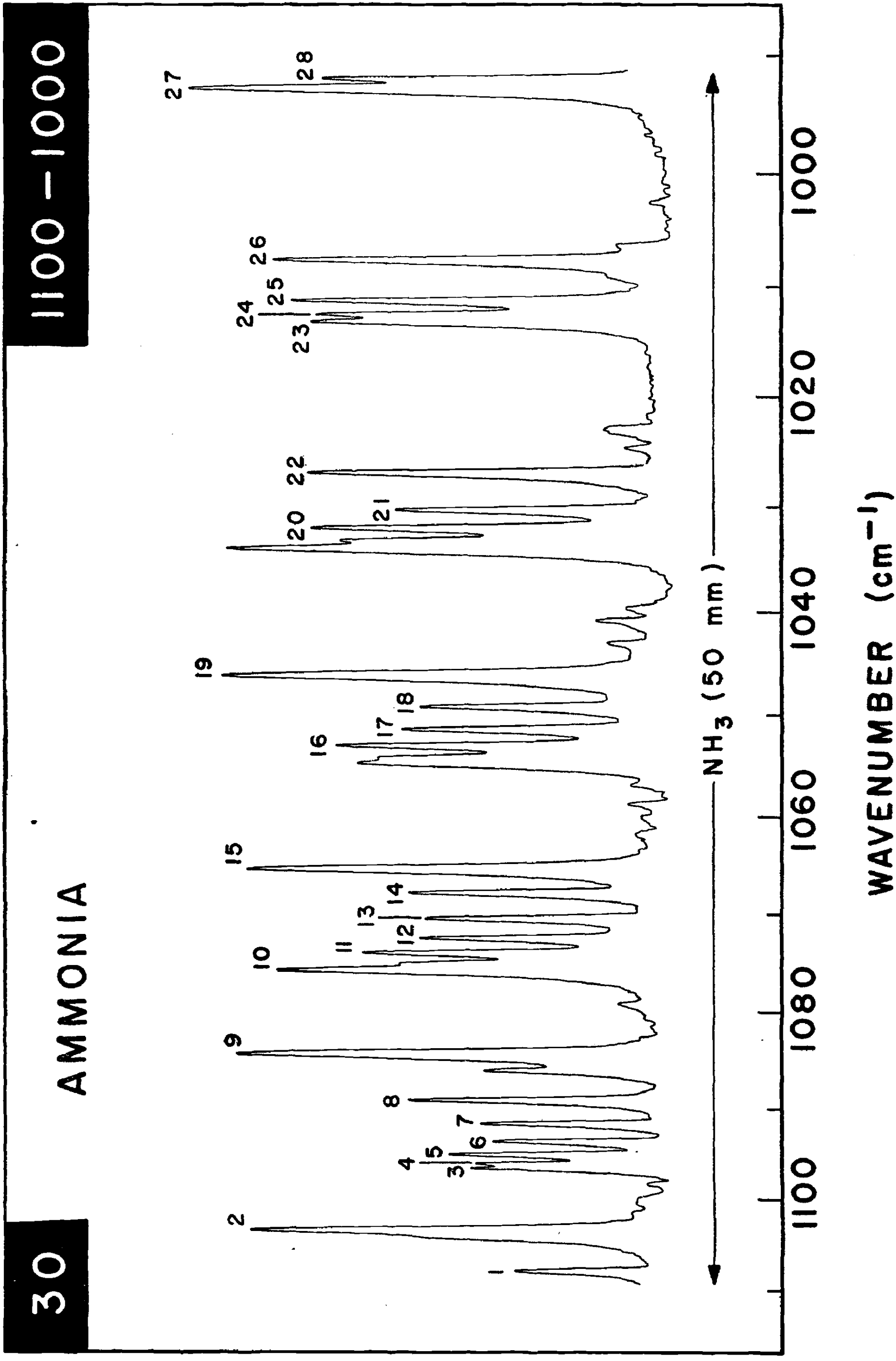

30
1100 — 1000
AMMONIA
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
NH_3 (50 mm)
1100
1080
1060
1040
1020
1000
WAVENUMBER (cm^{-1})

Chart 30. Ammonia (50 mm): 1100–1000 cm^{-1}

Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	1107·8$_5$	15	1065·5$_5$†‡
2	1103·4$_5$†‡	16	1053·1$_5$†
3	1096·7	17	1051·5
4	1096·1$_5$	18	1049·3$_5$
5	1095·1$_5$†	19	1046·4†‡
6	1093·7$_5$	20	1032·1$_5$†
7	1091·8$_5$	21	1030·4
8	1089·4†	22	1027·0$_5$†‡
9	1084·6†‡	23	1013·2
10	1075·9$_5$(b)	24	1012·4$_5$
11	1074·1$_5$†	25	1011·2†
12	1072·6$_5$	26	1007·5$_5$†‡
13	1070·6†	27	992·6†(b)
14	1068·0	28	991·7†

Resolution tests:
Line no. 3–line no. 4:0·55 cm^{-1}
Line no. 23–line no. 24:0·75 cm^{-1}
Line no. 10–line no. 11:1·8 cm^{-1}

† Part I calibration band.
‡ Suitable for use under lower resolution (*Chart 30A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) Blend of two component lines.

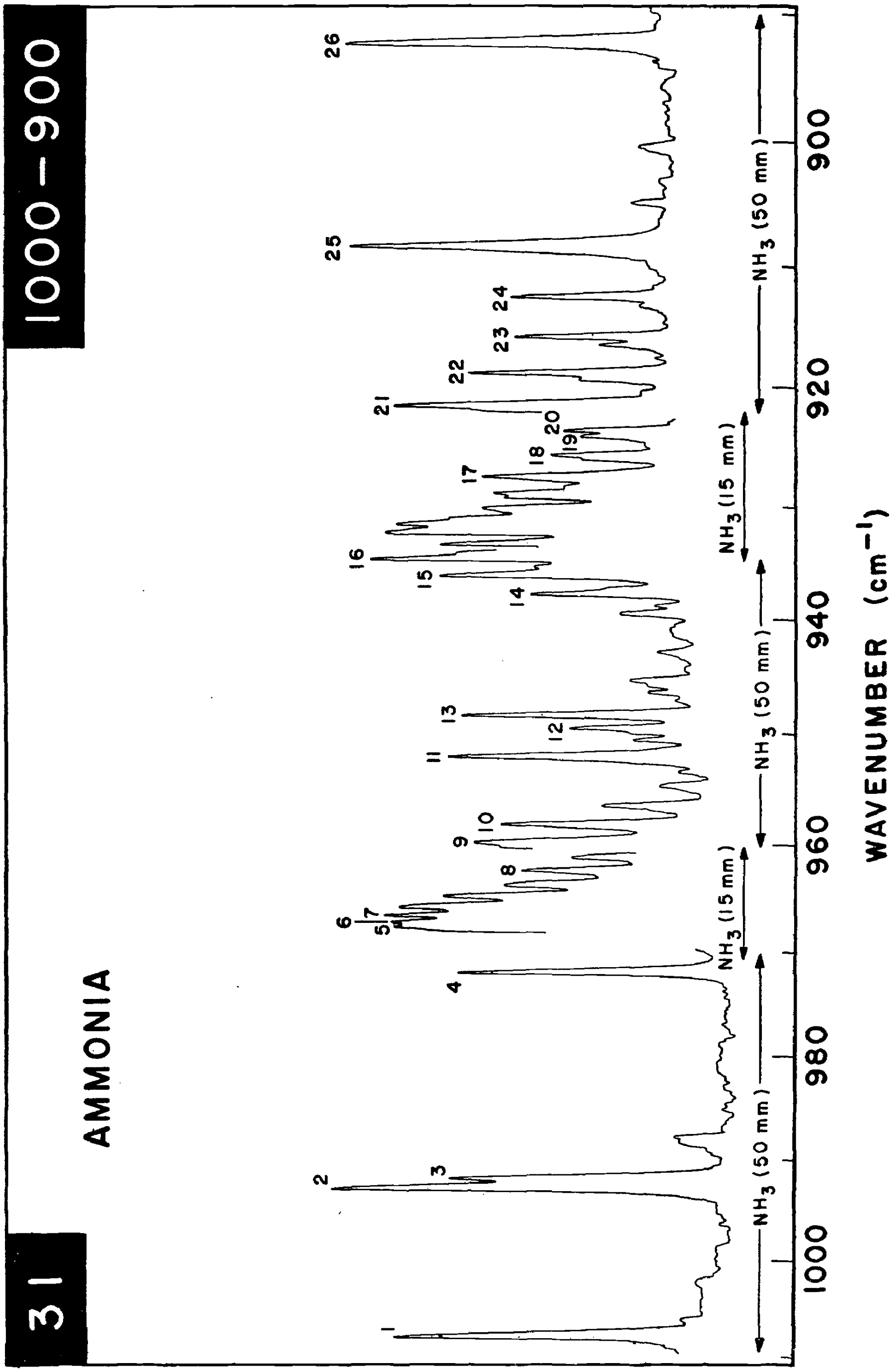

31
1000–900
AMMONIA
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
NH$_3$ (50 mm)
NH$_3$ (15 mm)
NH$_3$ (50 mm)
NH$_3$ (15 mm)
NH$_3$ (50 mm)
1000
980
960
940
920
900
WAVENUMBER (cm^{-1})

Chart 31. Ammonia (50 mm) and (15 mm): 1000–900 cm^{-1}

Ammonia (50 mm)		*Ammonia* (15 mm)	
Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	1007·5$_5$†‡	5	967·3$_5$
2	992·6†(b)	6	966·8
3	991·7†	7	966·2$_5$
4	971·9†‡		
....	......	....	.....
9	959·5	17	927·3
10	957·8$_5$	18	925·6
11	951·8†‡	19	924·0$_5$
12	949·3$_5$	20	923·6
13	948·2$_5$†		
14	937·6		
15	935·9†		
16	934·3		
....	......		
21	921·2$_5$		
22	918·6†		
23	915·7		
24	912·4‡		
25	908·2†‡		
26	892·0$_5$†‡(b)		

Resolution tests: Line no. 19–line no. 20: 0·45 cm^{-1}
Line no. 5–line no. 6: 0·55 cm^{-1}
Line no. 2–line no. 3: 0·9 cm^{-1}
Line no. 12–line no. 13: 1·1 cm^{-1}

† Part I calibration band.
‡ Suitable for use under lower resolution (*Chart 31A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) Blend of two component lines.

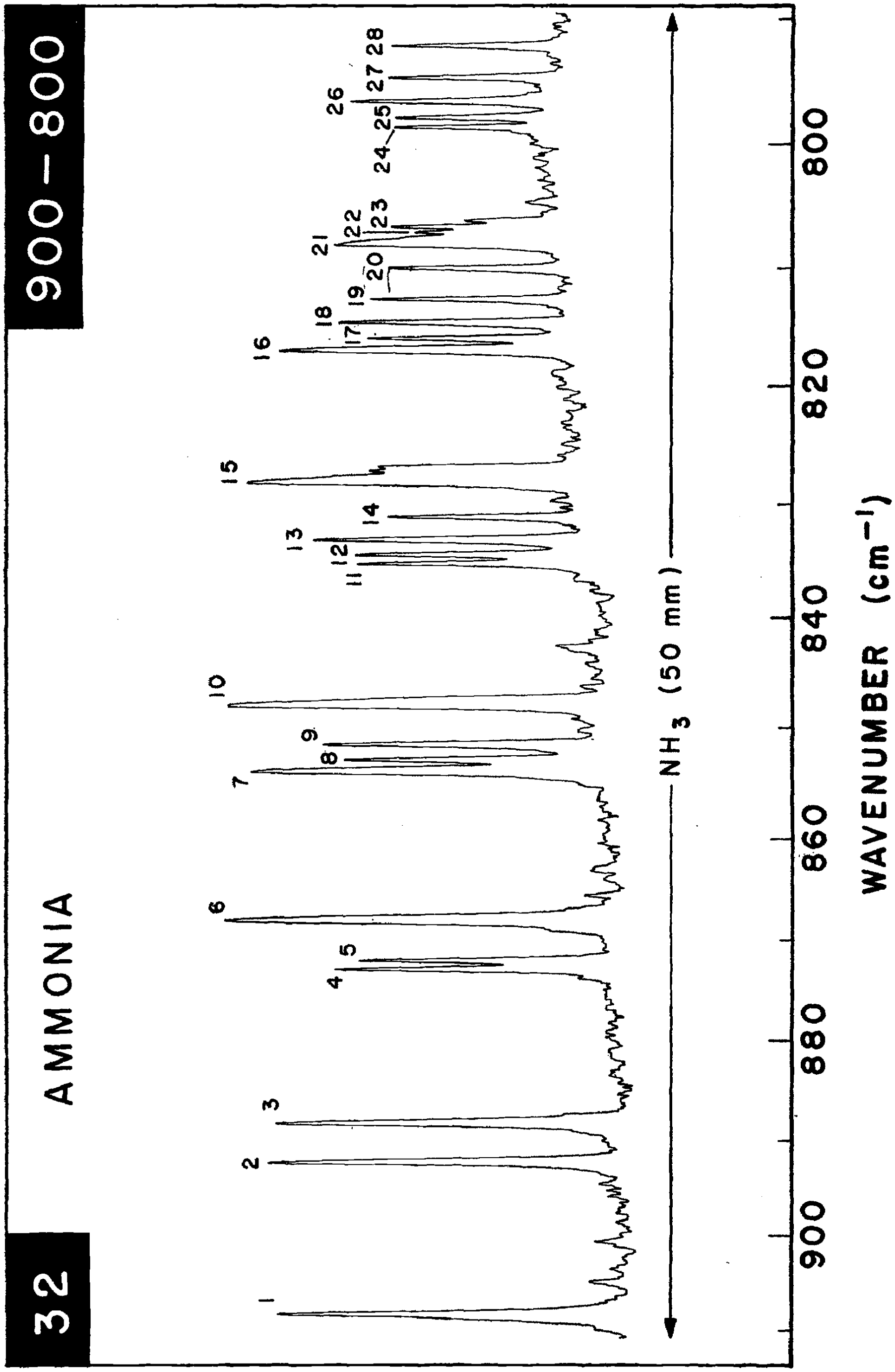

900 – 800
32
AMMONIA
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
NH$_3$ (50 mm)
900
880
860
840
820
800
WAVENUMBER (cm^{-1})

Chart 32. Ammonia (50 mm): 900–800 cm^{-1}

Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	908·2†‡	16	816·5$_5$‡(b)
2	892·0$_5$†‡(b)	17	815·6
3	888·0†‡	18	814·2$_5$†
4	872·6†	19	812·3
5	871·7$_5$†	20	809·7†
6	867·8†‡(c)	21	807·5(c)
7	853·7	22	806·7$_5$
8	852·7$_5$	23	806·2$_5$
9	851·3$_5$†	24	798·2$_5$
10	847·7‡(b)	25	797·4$_5$
11	834·8$_5$†	26	796·1$_5$†
12	834·0	27	794·2$_5$
13	832·6$_5$	28	791·7$_5$†‡
14	830·7†		
15	827·7$_5$(b)		

Resolution tests:
Line no. 22–line no. 23: 0·5 cm^{-1}
Line no. 4–line no. 5: 0·85 cm^{-1}
Line no. 16–line no. 17: 0·95 cm^{-1}

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 32A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) Blend of two component lines.
(c) Blend of three component lines.

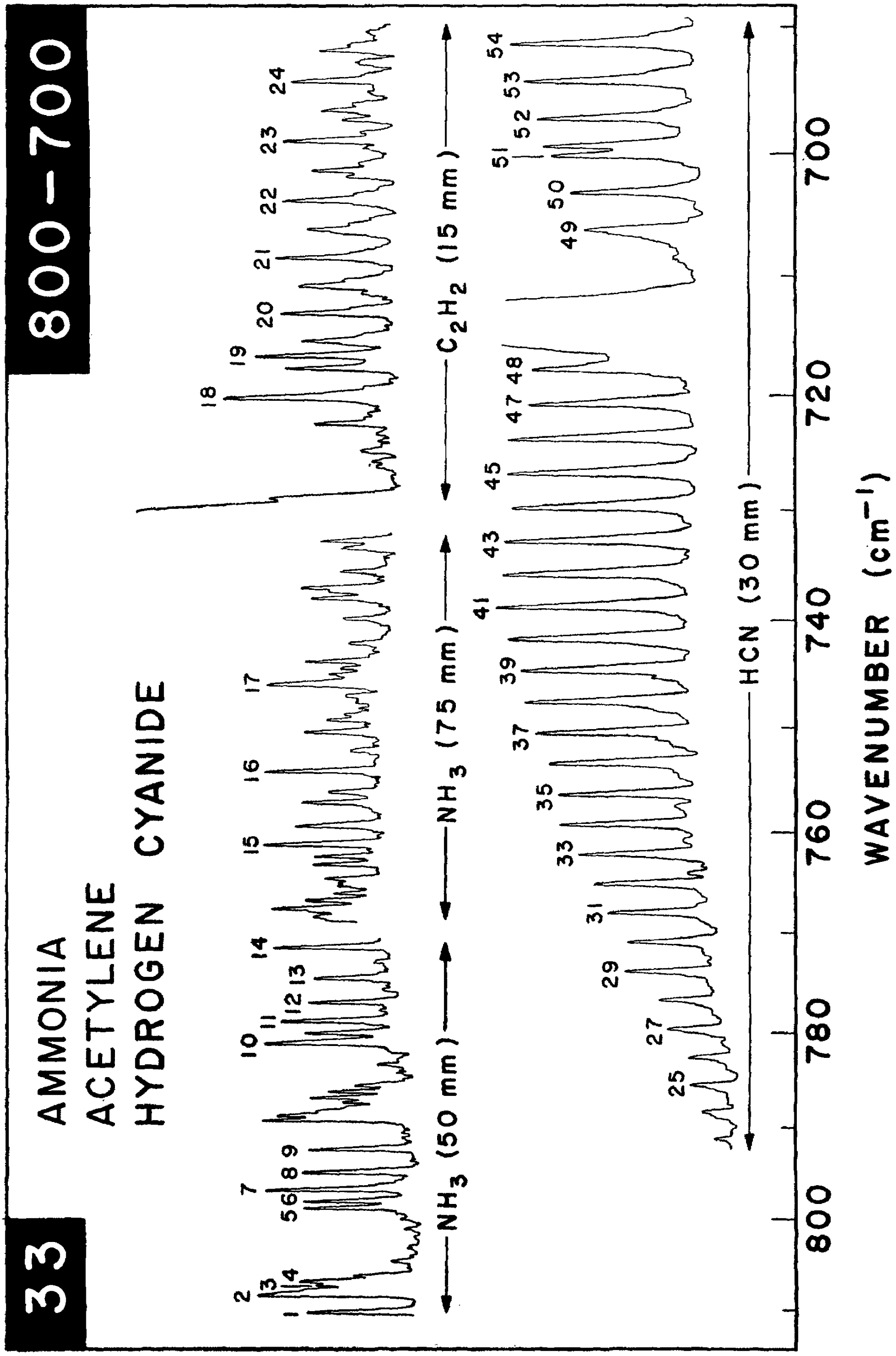

33
800–700
AMMONIA
ACETYLENE
HYDROGEN CYANIDE
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
25 27 29 31 33 35 37 39 41 43 45 47 48 49 50 51 52 53 54
NH_3 (50 mm)
NH_3 (75 mm)
C_2H_2 (15 mm)
HCN (30 mm)
800
780
760
740
720
700
WAVENUMBER (cm^{-1})

Chart 33. Ammonia (50 mm), (75 mm), acetylene (15 mm) and hydrogen cyanide (30 mm): 800–700 cm^{-1}

Ammonia (50 mm)		*Acetylene* (15 mm)		*Hydrogen cyanide* (30 mm)			
Line no.	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})	*Line no.*	*Wavenumber*(a) (vac.) (cm^{-1})
1	809·7†	18	719·9‡	25	785·5$_5$†‡	40	741·5†‡
2	807·5(c)	19	716·3$_5$	26	782·6$_5$†‡	41	738·5$_5$†‡
3	806·7$_5$	20	712·6$_5$‡	27	779·7$_5$†‡	42	735·6†‡
4	806·2$_5$	21	707·9$_5$‡	28	776·8†‡	43	732·6$_5$†‡
5	798·2$_5$	22	703·2$_5$‡	29	773·8$_5$†‡	44	729·7†‡
6	797·4$_5$	23	698·5‡	30	770·9$_5$†‡	45	726·7$_5$†‡
7	796·1$_5$†	24	693·8‡	31	768·0†‡	46	723·8†‡
8	794·2$_5$			32	765·0$_5$†‡	47	720·8$_5$†‡
9	791·7$_5$†‡			33	762·1$_5$†‡	48	717·9†
10	780·4(b)			34	759·2†‡	49	706·0$_5$†‡
11	778·3†‡			35	756·2$_5$†‡	50	703·1†‡
12	776·5			36	753·3†‡	51	700·1$_5$†
13	774·0			37	750·3$_5$†‡	52	697·2†‡
14	770·9†‡			38	747·4†‡	53	694·2$_5$†‡
				39	744·4$_5$†‡	54	691·3†‡
Ammonia (75 mm)							
15	760·7†‡						
16	753·6†						
17	745·4(c)						

Resolution tests: Line no. 3–line no. 4: 0·5 cm^{-1}
Line no. 29–line no. 30: 2·9 cm^{-1}
Line no. 53–line no. 54: 2·95 cm^{-1}

† Part I calibration band.
‡ Suitable for use under lower resolution (*Chart 33A*).
(a) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(b) Blend of two component lines.
(c) Blend of three component lines.

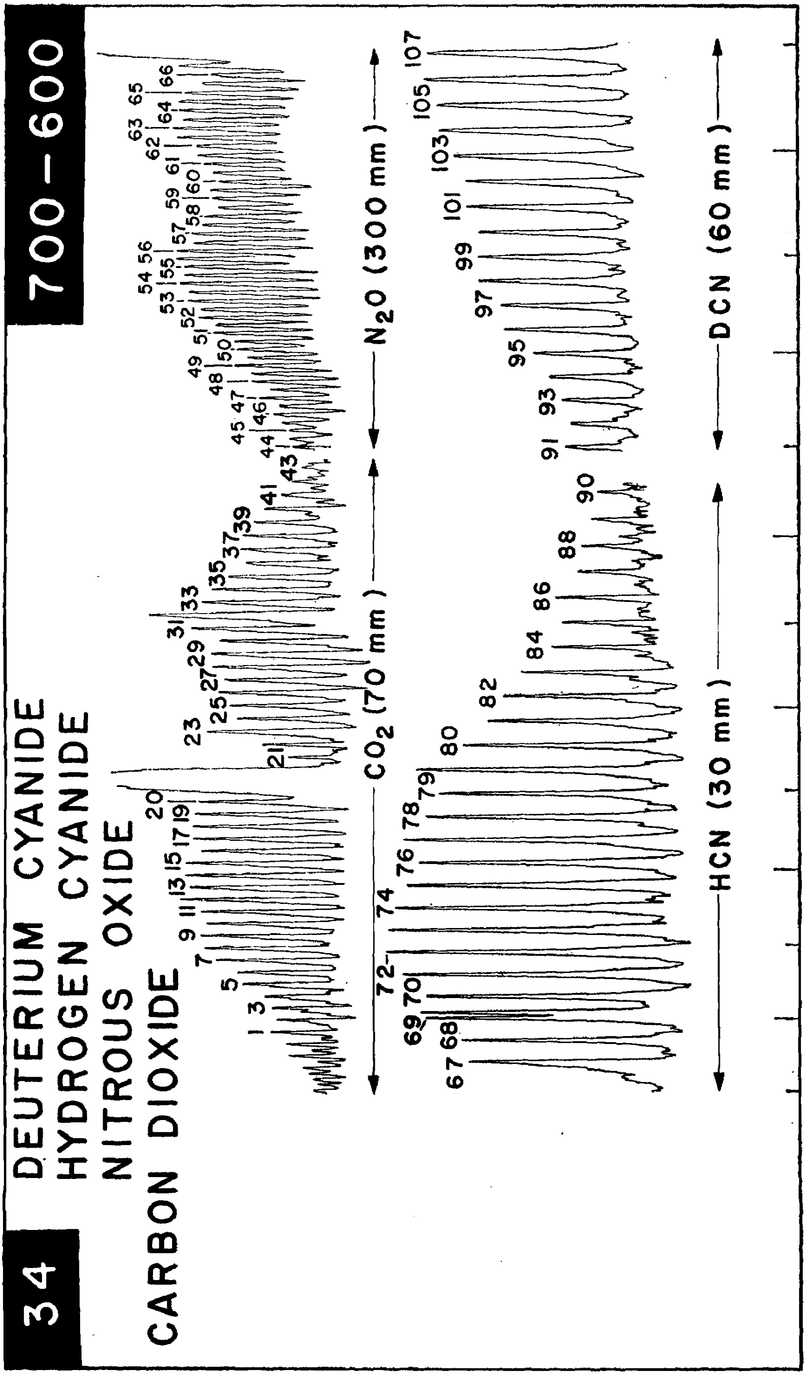

34
DEUTERIUM CYANIDE
HYDROGEN CYANIDE
NITROUS OXIDE
CARBON DIOXIDE
700 – 600
CO2 (70 mm)
N2O (300 mm)
HCN (30 mm)
DCN (60 mm)
1 3 5 7 9 11 13 15 17 19 20 21 23 25 27 29 31 33 35 37 39 41 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66
67 68 69 70 72 74 76 78 79 80 82 84 86 88 90 91 93 95 97 99 101 103 105 107
700
680
660
640
620
600
WAVENUMBER (cm⁻¹)

Chart 34. Carbon dioxide (70 mm), nitrous oxide (300 mm)[(a)], hydrogen cyanide (30 mm) and deuterium cyanide (60 mm): 700–600 cm^{-1}

Carbon dioxide (70 mm)				*Nitrous oxide* (300 mm)			
Line no.	*Wavenumber*[(b)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(b)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(b)] (vac.) (cm^{-1})	*Line no.*	*Wavenumber*[(b)] (vac.) (cm^{-1})
1	701·7†‡	24	661·1$_5$†‡	44	630·1$_5$	57	608·1$_5$†
2	700·0$_5$†‡	25	659·6†‡	45	628·4$_5$†	58	606·4$_5$†
3	698·4$_5$†‡	26	658·0$_5$†‡	46	626·7$_5$†	59	604·7$_5$†
4	696·8†‡	27	656·5$_5$†‡	47	625·0$_5$†	60	603·0$_5$†
5	695·2†‡	28	655·0†‡	48	623·3$_5$†	61	601·4†
6	693·6†‡	29	653·5†‡	49	621·7†	62	599·7†
7	692·0†‡	30	651·9$_5$†‡	50	620·0†	63	598·0$_5$†
8	690·3$_5$†‡	31	650·4†‡	51	618·3†	64	596·3$_5$†
9	688·8†‡	32	648·9†‡	52	616·6†	65	594·6$_5$†
10	687·1$_5$†‡	33	647·4†‡	53	614·9†	66	592·9$_5$†
11	685·5$_5$†‡	34	645·9†‡	54	613·2†		
12	683·9$_5$†‡	35	644·3$_5$†‡	55	611·5†		
13	682·4†‡	36	642·8$_5$†‡	56	609·8†		
14	680·8†‡	37	641·3$_5$†‡				
15	679·2†‡	38	639·8$_5$†‡				
16	677·6†‡	39	638·3$_5$†‡				
17	676·0$_5$†‡	40	636·8$_5$†‡				
18	674·4$_5$†‡	41	635·4†				
19	672·9†‡	42	633·9†				
20	671·3$_5$†‡	43	632·4†				
21	665·8$_5$†						
22	664·3†						
23	662·7†‡						

(continued overleaf)

Chart 34 (continued)

Hydrogen cyanide (30 mm)				Deuterium cyanide (60 mm)	
Line no.	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})	*Line no.*	*Wavenumber*$^{(b)}$ (vac.) (cm^{-1})
67	706·0$_5$†‡	80$^{(c)}$	664·7†‡	91	630·1
68	703·1†‡	81	661·7$_5$†‡	92	627·6$_5$
69	700·1$_5$†	82	658·8†‡	93	625·2
70	697·2†‡	83	655·8$_5$†‡	94	622·6$_5$
71	694·2$_5$†‡	84	652·9†‡	95	620·3‡
72	691·3†‡	85	649·9†	96	617·8‡
73	688·3$_5$†‡	86	647·0†	97	615·3$_5$‡
74	685·3$_5$†‡	87	644·0$_5$†	98	612·8$_5$‡
75	682·4†‡	88	641·1†	99	610·4$_5$‡
76	679·4$_5$†‡	89	638·1$_5$†	100	608·0‡
77	676·5†‡	90	635·2	101	605·5$_5$‡
78	673·5$_5$†‡			102	603·1‡
79$^{(c)}$	670·6†			103	600·6‡
				104	598·2$_5$‡
				105	595·8‡
				106	593·3‡
				107	590·9‡

Resolution tests: The individual band spacing in the nitrous oxide spectrum is approx. 0·85 cm^{-1}
Line no. 13–line no. 14: 1·6 cm^{-1}
Line no. 99–line no. 100: 2·45 cm^{-1}
Line no. 74–line no. 75: 2·95 cm^{-1}

---

† Part I calibration line.
‡ Suitable for use under lower resolution (*Chart 34A*).
(a) Note that alternate lines are omitted.
(b) The estimated uncertainty does not exceed ±0·1 cm^{-1}.
(c) Note that the line following no. 79 is omitted; it is superimposed on the *Q*-branch of carbon dioxide.

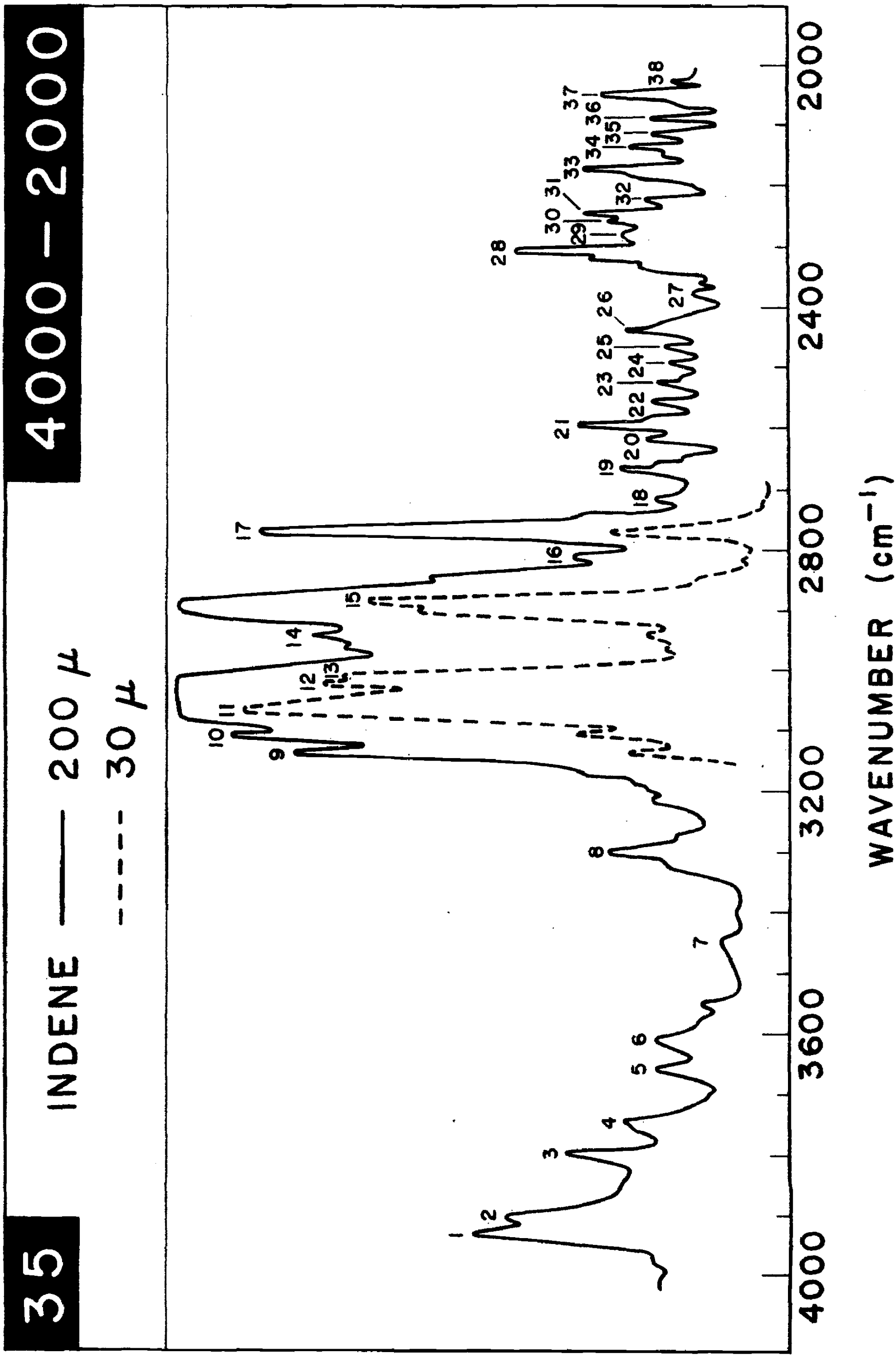

35
4000 – 2000
INDENE —— 200 μ
- - - - 30 μ
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
4000
3600
3200
2800
2400
2000
WAVENUMBER (cm⁻¹)

Chart 35. Indene (liquid film)(a): 4000–2000 cm^{-1}

Band no.	*Wavenumber* (vac.) (cm^{-1})	*Band no.*	*Wavenumber* (vac.) (cm^{-1})	*Band no.*	*Wavenumber* (vac.) (cm^{-1})
1	3926·5 ± 1	13	3015·0 ± 0·5*	25	2465·6 ± 0·5* §
2	3900·7 ± 0·5*	14	2943·8 ± 1*	26	2439·5 ± 1 §
3	3797·5 ± 1	15	2887·0 ± 1	27	2379·0 ± 1* §
4	3747·5 ± 2* §	16	2812·5 ± 1*	28	2304·8 ± 0·5
5	3656·7 ± 1 §	17	2771·0 ± 0·5	29	2271·5 ± 0·5* §
6	3610·0 ± 2 §	18	2718·0 ± 1* §	30	2258·0 ± 0·5* §
7	3455·0 ± 3 §	19	2673·7 ± 1	31	2243·7 ± 0·5 §
8	3297·0 ± 1·5	20	2622·3 ± 0·5*	32	2223·0 ± 2* §
9	3139·5 ± 1*	21	2598·6 ± 0·5	33	2172·8 ± 0·5
10	3110·0 ± 1*	22	2558·5 ± 1 §	34	2135·8 ± 0·5
11	3068·5 ± 2·5 §	23	2525·9 ± 0·5	35	2113·5 ± 0·5
12	3025·6 ± 0·5*	24	2490·3 ± 0·5* §	36	2090·2 ± 0·5
				37	2049·6 ± 0·5
				38	2027·4 ± 0·5* §

§ Because of asymmetry, superposition on atmospheric water vapour or carbon dioxide lines, or for other reasons, these bands are less satisfactory; they are included to provide secondary calibration points in regions where better bands are not available.

* These bands may not be resolved by smaller prism spectrometers.

(a) The indene should be sealed in glass ampoules immediately after distillation and used only from freshly opened ampoules.

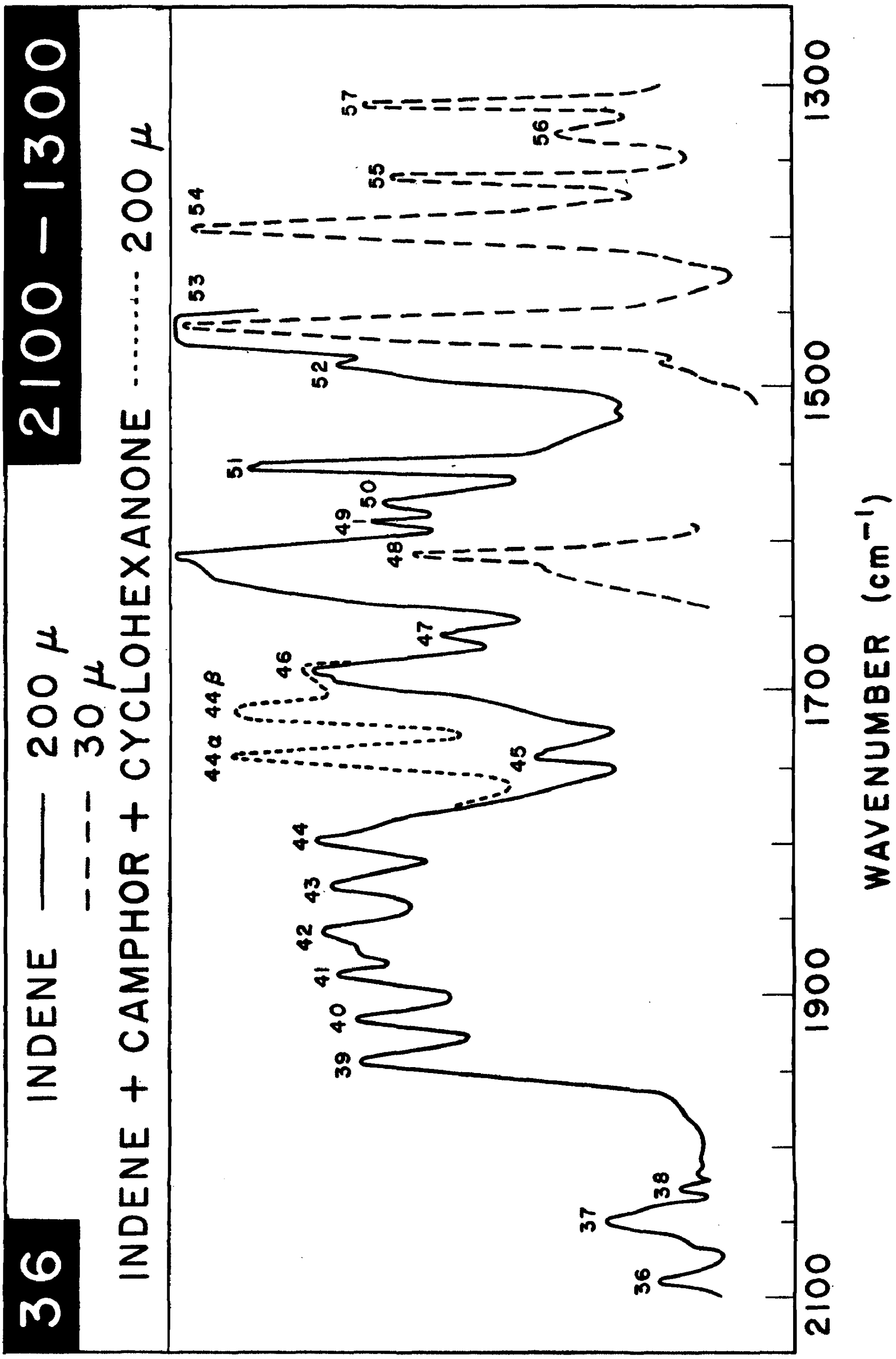

36
2100 – 1300
INDENE —— 200 μ
- - - - 30 μ
INDENE + CAMPHOR + CYCLOHEXANONE ········ 200 μ
36
37
38
39
40
41
42
43
44
44α
44β
45
46
47
48
49
50
51
52
53
54
55
56
57
2100
1900
1700
1500
1300
WAVENUMBER (cm^{-1})

Chart 36. Indene (liquid film)(a): 2100–1300 cm^{-1}

Band no.	*Wavenumber* (vac.) (cm^{-1})	*Band no.*	*Wavenumber* (vac.) (cm^{-1})
36	2090·2 ± 0·5	47	1661·5 ± 0·5 §
37	2049·6 ± 0·5	48	1609·6 ± 0·2
38	2027·4 ± 0·5* §	49	1587·7 ± 0·2
39	1943·2 ± 0·5	50	1574·3 ± 0·5 §
40	1915·0 ± 0·3	51	1553·3 ± 0·5 §
41	1884·5 ± 0·5	52	1483·2 ± 0·5* §
42	1856·7 ± 0·3	53	1457·8 ± 0·5
43	1825·5 ± 0·5	54	1393·2 ± 1 §
44	1796·9 ± 0·3	55	1361·3 ± 0·4
44α	1741·8 ± 0·5 (camphor)(b)	56	1332·5 ± 0·5 §
44β	1713·5 ± 1 (cyclohexanone)(b)	57	1312·5 ± 0·3
45	1738·2 ± 1 §		
46	1686·0 ± 2 §		

§, *, (a) See footnotes to *Chart 35.*

(b) To overcome a lack of suitable calibration points in the indene spectrum between bands no. 44 and 47 it is suggested that 0·8 weight per cent of camphor and cyclohexanone be added. These additives introduce the additional bands no. 44α and 44β. They do not significantly displace any of the indene bands outside the region 1780–1690 cm^{-1} nor do they introduce any extra bands in other regions of the spectrum. They have no deleterious effect on the chemical stability of indene.

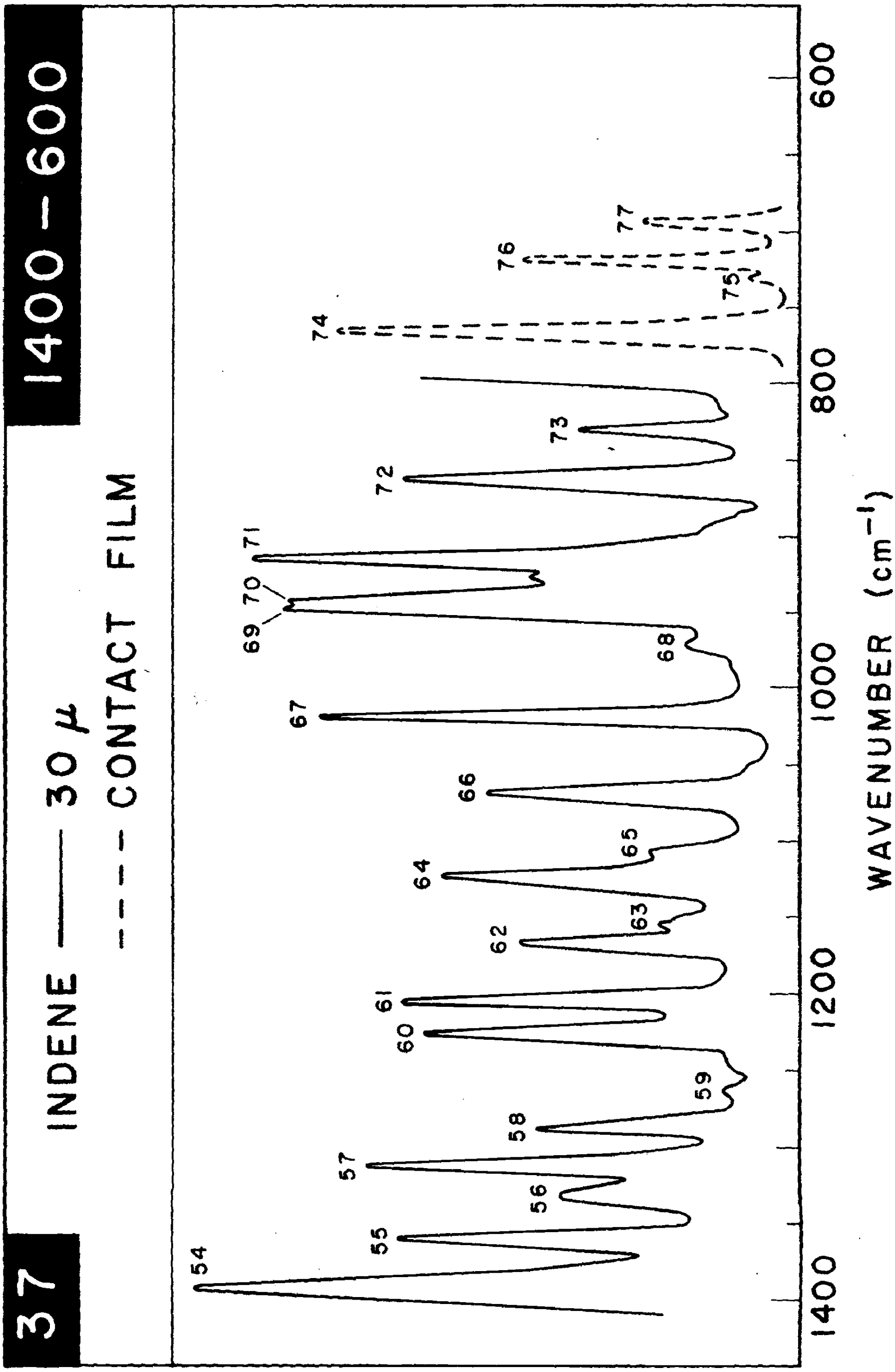

37
1400 – 600
INDENE ——— 30 μ
- - - - CONTACT FILM
54
55
56
57
58
59
60
61
62
63
64
65
66
67
68
69
70
71
72
73
74
75
76
77
1400
1200
1000
800
600
WAVENUMBER (cm⁻¹)

Chart 37. Indene (liquid film)(a): 1400–600 cm^{-1}

Band no.	*Wavenumber* (vac.) (cm^{-1})	*Band no.*	*Wavenumber* (vac.) (cm^{-1})
54	1393·2 ± 1 §	66	1067·9 ± 0·2
55	1361·3 ± 0·4	67	1018·6 ± 0·2
56	1332·5 ± 0·5 §	68	972·0 ± 0·5* §
57	1312·5 ± 0·3	69	947·2 ± 0·3 §
58	1287·8 ± 0·2	70	942·3 ± 0·3* §
59	1263·8 ± 0·5* §	71	914·8 ± 0·2
60	1226·2 ± 0·2	72	861·3 ± 0·2
61	1205·2 ± 0·2	73	830·5 ± 0·2
62	1166·2 ± 0·3	74	765·4 ± 0·5
63	1154·5 ± 0·5* §	75	730·1 ± 0·2
64	1122·7 ± 0·2 §	76	718·2 ± 0·3
65	1106·4 ± 0·5* §	77	692·8 ± 0·7 §

§, *, (a) See footnotes to *Chart 35.*

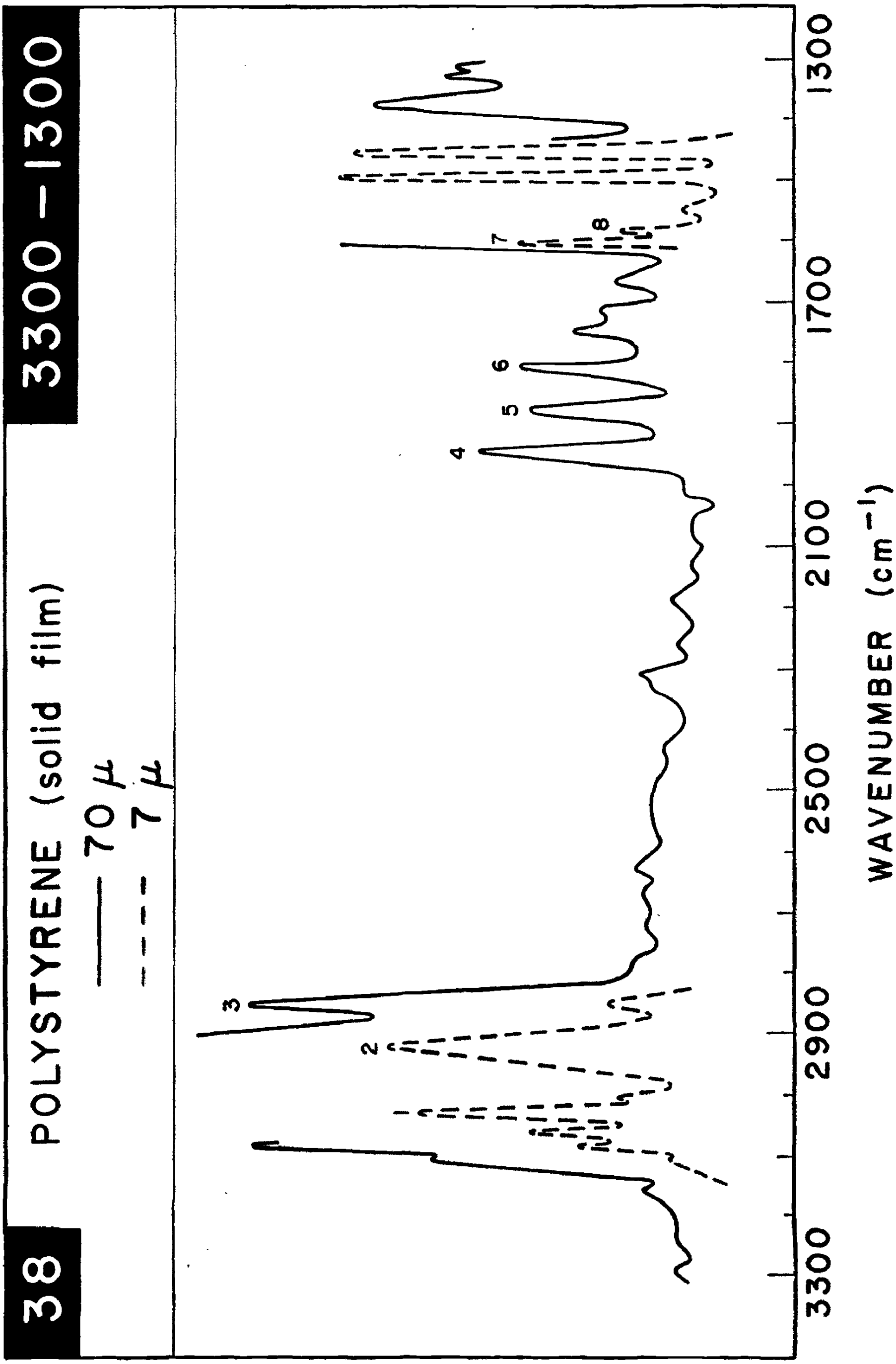

38
3300 – 1300
POLYSTYRENE (solid film)
—— 70 μ
- - - - 7 μ
2
3
4
5
6
7
8
3300
2900
2500
2100
1700
1300
WAVENUMBER (cm^{-1})

Chart 38. Polystyrene (solid film)[(a)]: 3300–1300 cm^{-1}

Band no.	*Wavenumber* (vac.) (cm^{-1})
1	3027·1 ± 0·3
2	2924 ± 2
3	2850·7 ± 0·3
4	1944·0 ± 1
5	1871·0 ± 0·3
6	1801·6 ± 0·3
7	1601·4 ± 0·3
8	1583·1 ± 0·3

(a) Films from commercial sources of polystyrene frequently exhibit strong interference patterns; such films should be slightly bent or otherwise deformed before using for calibration purposes.

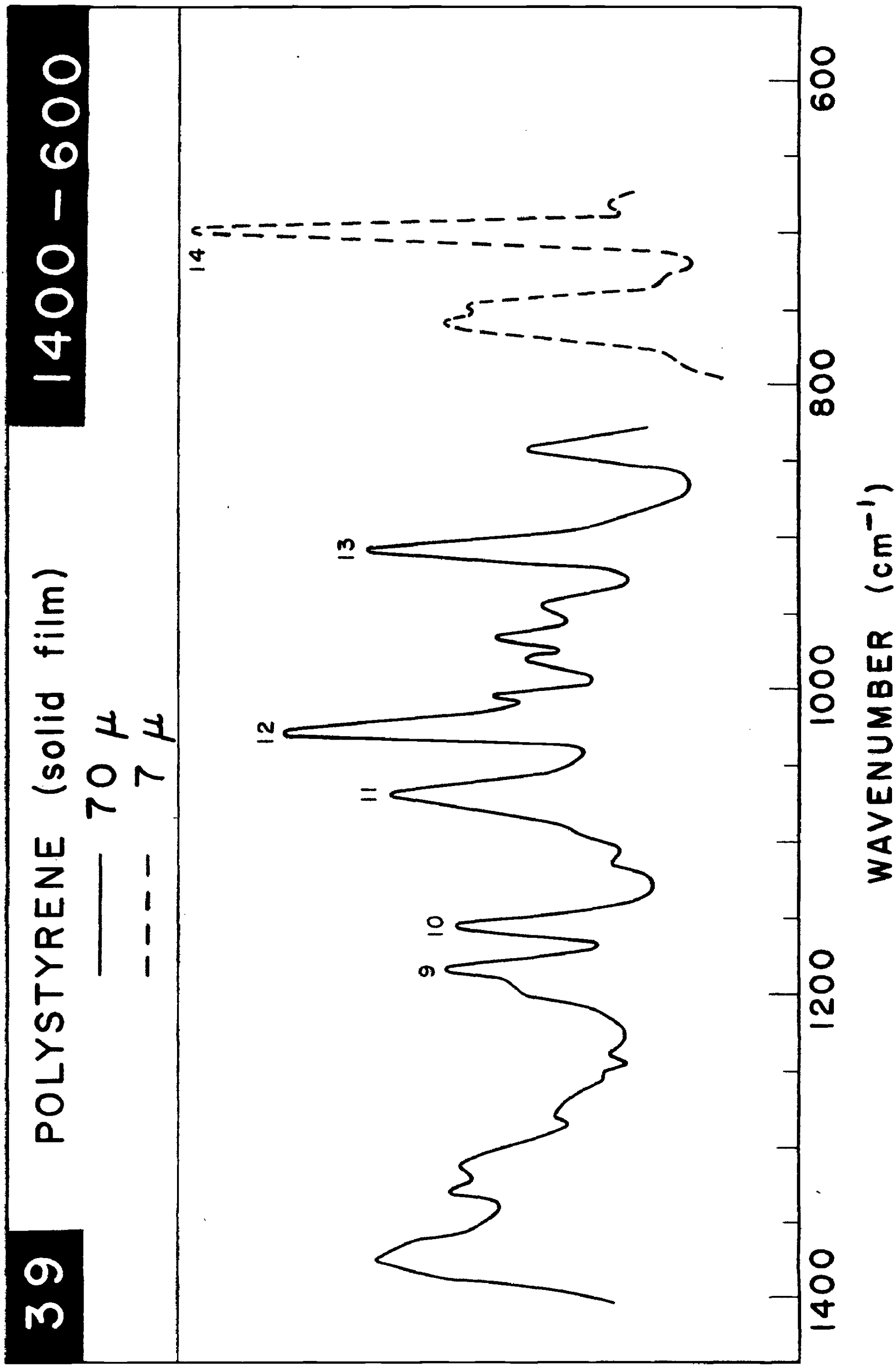
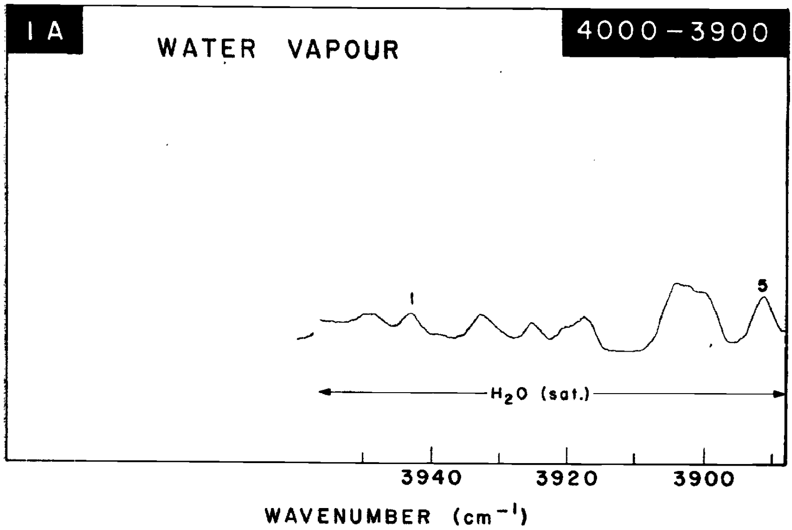
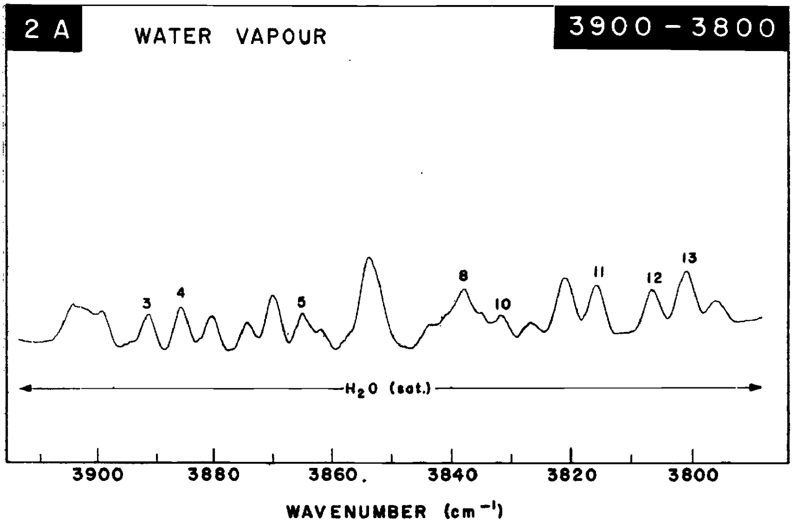

39
1400 – 600
POLYSTYRENE (solid film)
—— 70 μ
- - - - 7 μ
9
10
11
12
13
14
1400
1200
1000
800
600
WAVENUMBER (cm⁻¹)

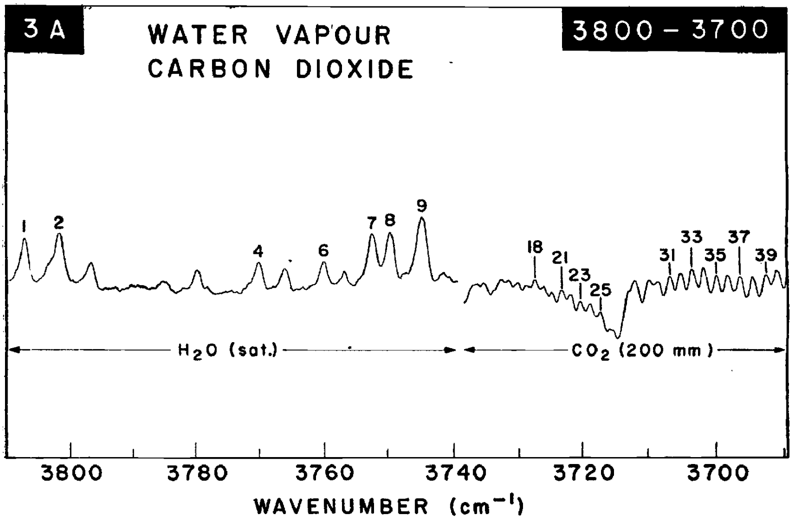
Chart 39. Polystyrene (solid film)[(a)]: 1400–600 cm^{-1}

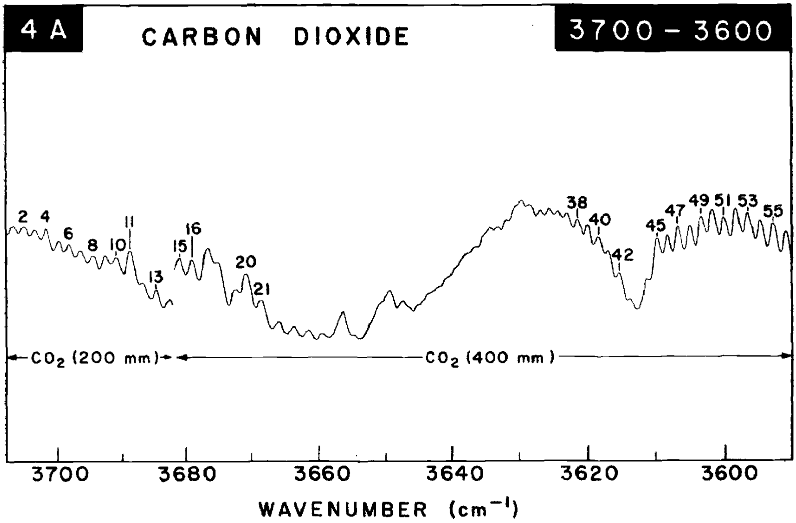
Band no.	*Wavenumber* (vac.) (cm^{-1})
9	1181·4 ± 0·3
10	1154·3 ± 0·3
11	1069·1 ± 0·3
12	1028·0 ± 0·3
13	906·7 ± 0·3
14	698·9 ± 0·5

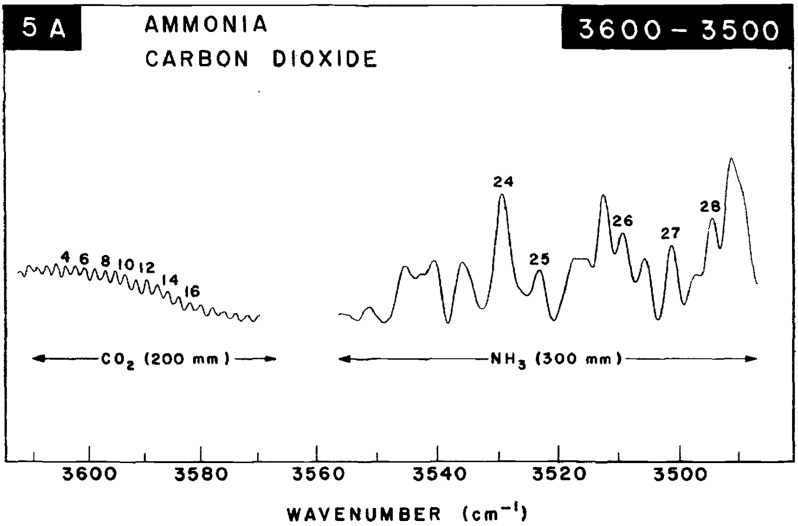
(a) See footnote to *Chart 38.*

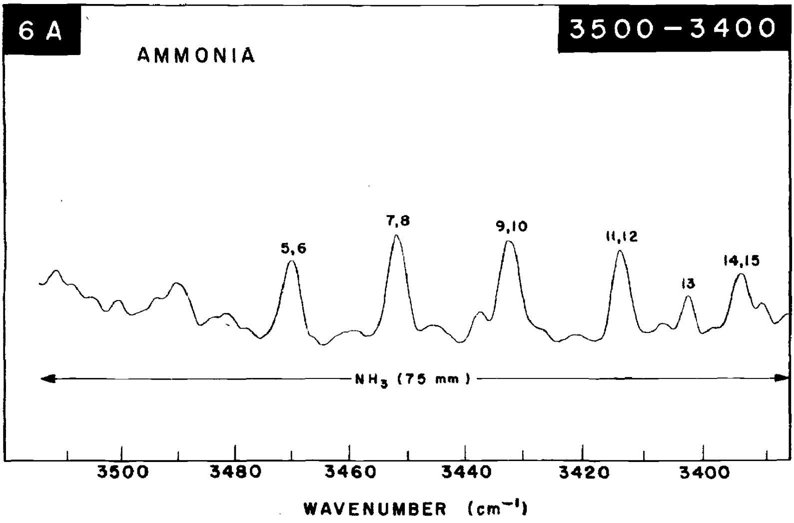

1 A
WATER VAPOUR
4000 – 3900
1
5
H2O (sat.)
3940
3920
3900
WAVENUMBER (cm⁻¹)

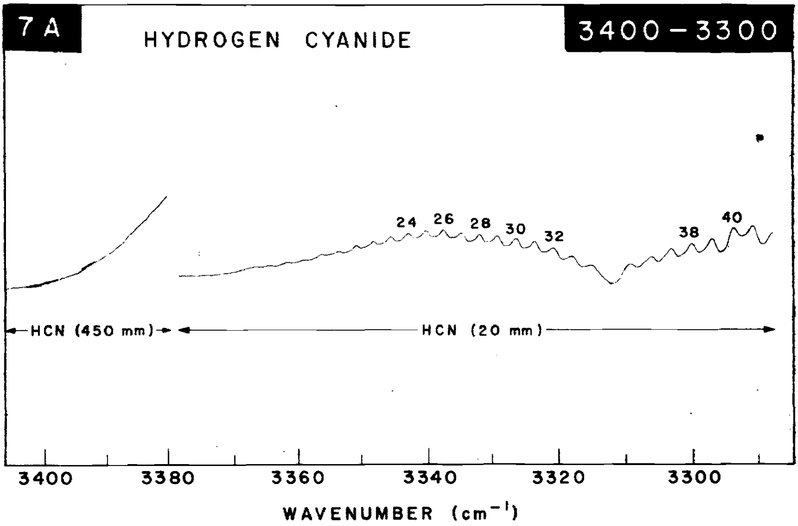

2 A
WATER VAPOUR
3900 – 3800
3
4
5
8
10
11
12
13
H2O (sat.)
3900
3880
3860
3840
3820
3800
WAVENUMBER (cm⁻¹)

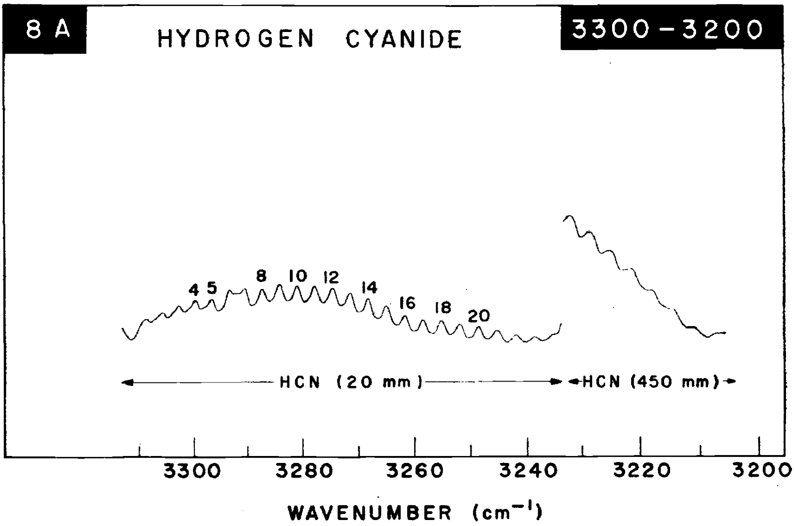

3 A
WATER VAPOUR
CARBON DIOXIDE
3800 – 3700
1
2
4
6
7
8
9
18
21
23
25
31
33
35
37
39
H2O (sat.)
CO2 (200 mm)
3800
3780
3760
3740
3720
3700
WAVENUMBER (cm⁻¹)

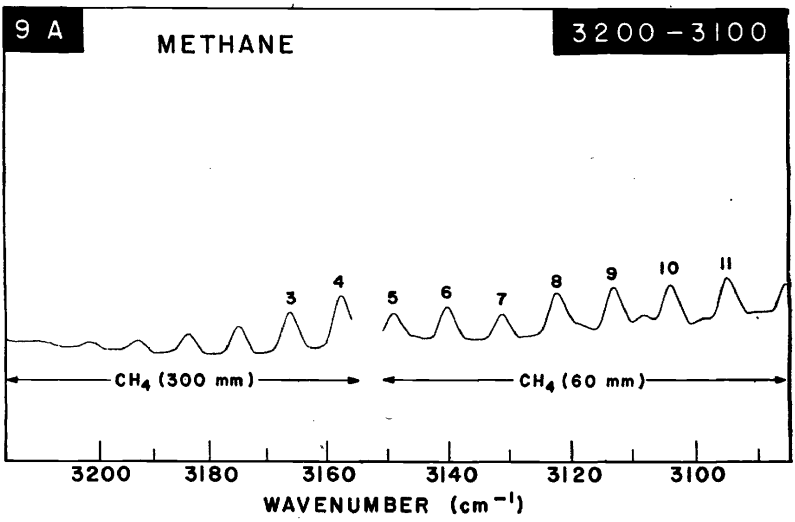

4 A
CARBON DIOXIDE
3700 - 3600
2 4 6 8 10 11 13 15 16 20 21
38 40 42 45 47 49 51 53 55
CO₂ (200 mm)
CO₂ (400 mm)
3700
3680
3660
3640
3620
3600
WAVENUMBER (cm⁻¹)

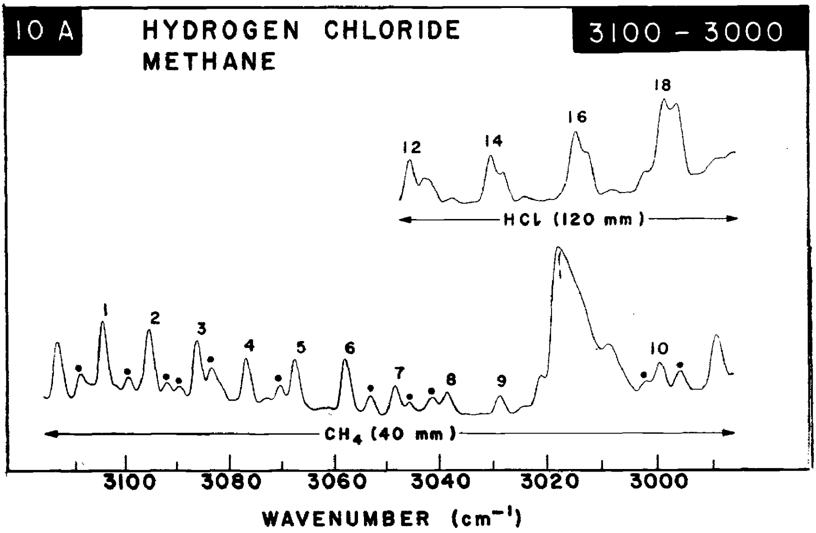

5 A
AMMONIA
CARBON DIOXIDE
3600 - 3500
4 6 8 10 12 14 16
24 25 26 27 28
CO₂ (200 mm)
NH₃ (300 mm)
3600
3580
3560
3540
3520
3500
WAVENUMBER (cm⁻¹)

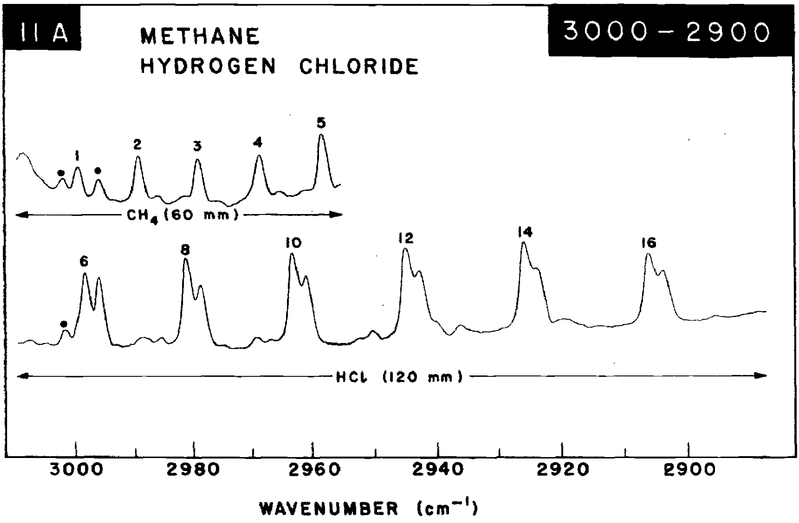

6 A
AMMONIA
3500 - 3400
5,6
7,8
9,10
11,12
13
14,15
NH₃ (75 mm)
3500
3480
3460
3440
3420
3400
WAVENUMBER (cm⁻¹)

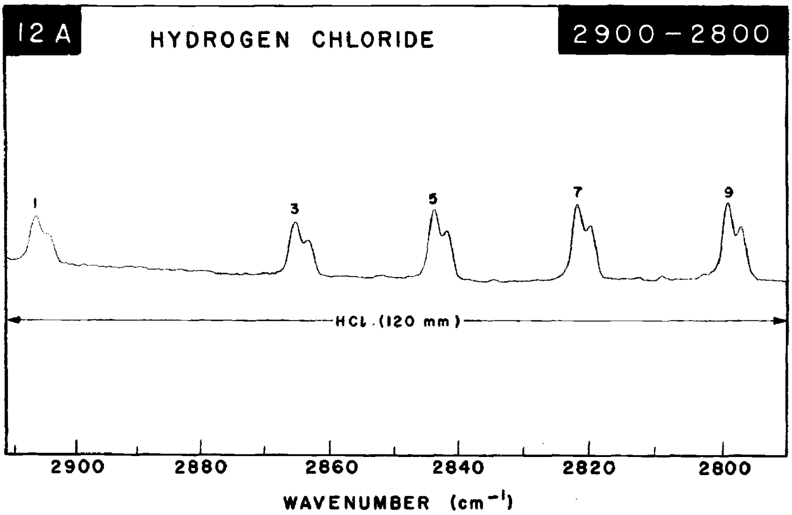

7 A
HYDROGEN CYANIDE
3400 – 3300
24
26
28
30
32
38
40
HCN (450 mm)
HCN (20 mm)
3400
3380
3360
3340
3320
3300
WAVENUMBER (cm⁻¹)

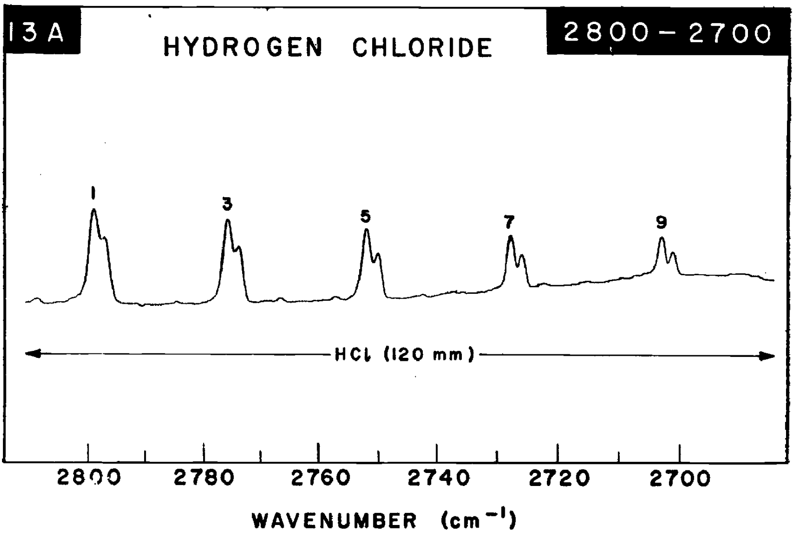

8 A
HYDROGEN CYANIDE
3300 – 3200
4
5
8
10
12
14
16
18
20
HCN (20 mm)
HCN (450 mm)
3300
3280
3260
3240
3220
3200
WAVENUMBER (cm⁻¹)

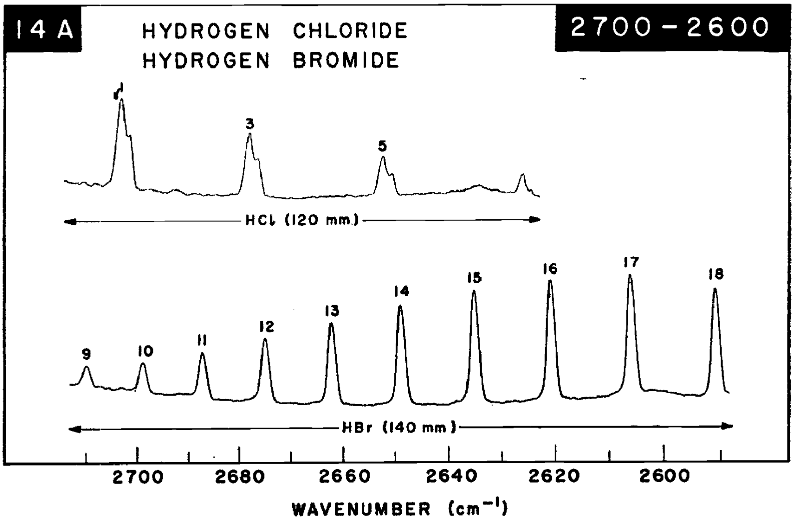

9 A
METHANE
3200 – 3100
3
4
5
6
7
8
9
10
11
CH₄ (300 mm)
CH₄ (60 mm)
3200
3180
3160
3140
3120
3100
WAVENUMBER (cm⁻¹)

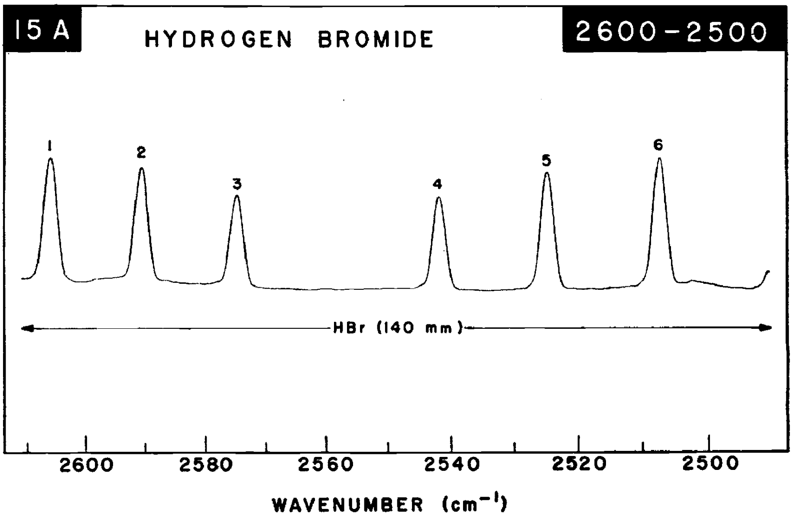

10 A
HYDROGEN CHLORIDE
METHANE
3100 - 3000
12
14
16
18
HCL (120 mm)
1
2
3
4
5
6
7
8
9
10
CH$_4$ (40 mm)
3100
3080
3060
3040
3020
3000
WAVENUMBER (cm^{-1})

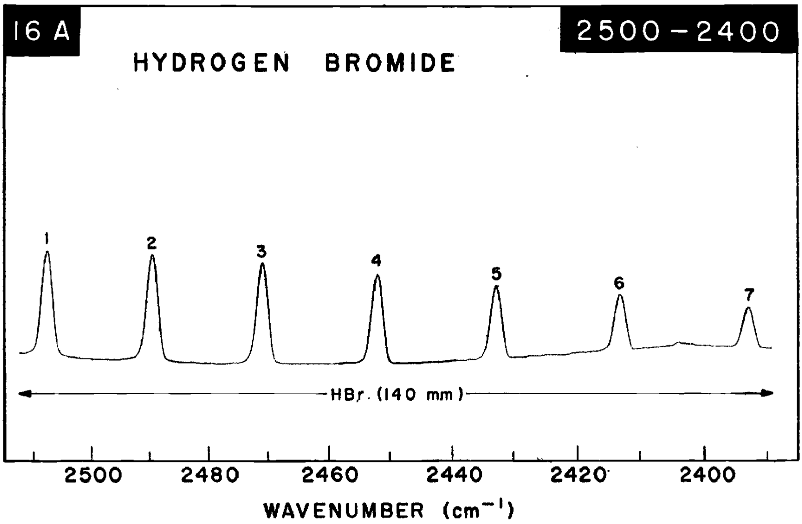

11 A
METHANE
HYDROGEN CHLORIDE
3000 - 2900
1
2
3
4
5
CH$_4$ (60 mm)
6
8
10
12
14
16
HCL (120 mm)
3000
2980
2960
2940
2920
2900
WAVENUMBER (cm^{-1})

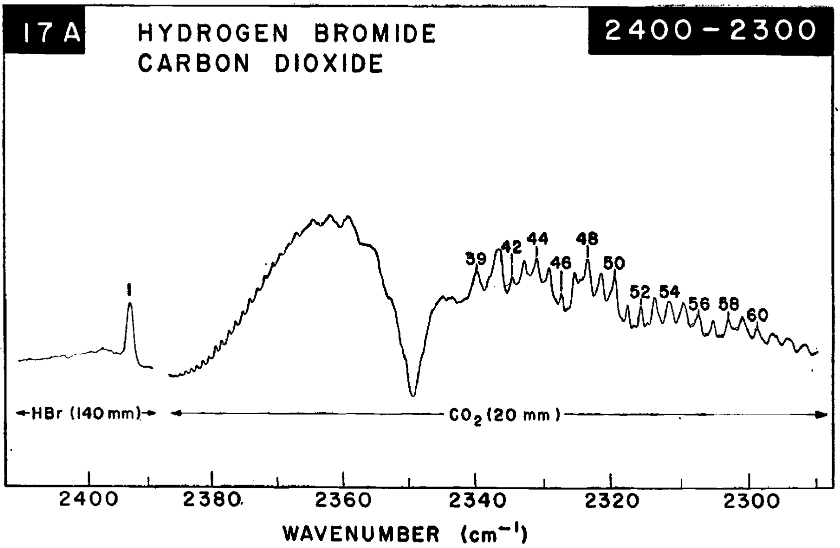

12 A
HYDROGEN CHLORIDE
2900 - 2800
1
3
5
7
9
HCL (120 mm)
2900
2880
2860
2840
2820
2800
WAVENUMBER (cm^{-1})

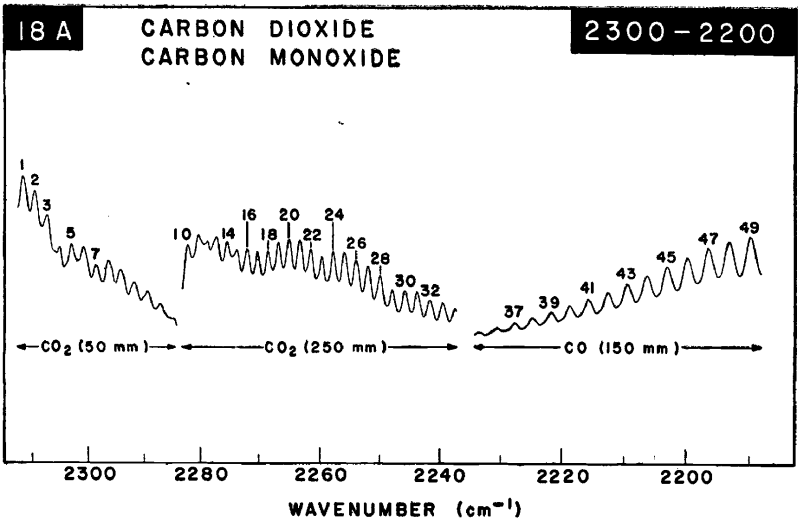

13 A
HYDROGEN CHLORIDE
2800 – 2700
1
3
5
7
9
HCl (120 mm)
2800
2780
2760
2740
2720
2700
WAVENUMBER (cm⁻¹)

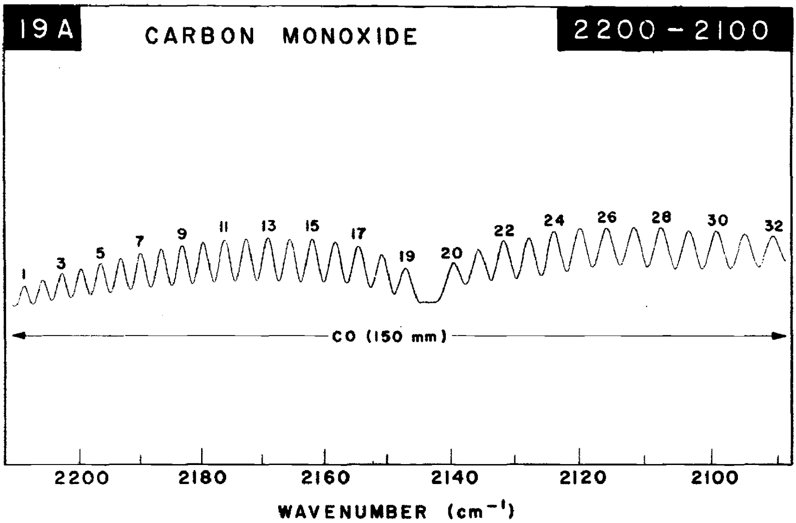

14 A
HYDROGEN CHLORIDE
HYDROGEN BROMIDE
2700 – 2600
1
3
5
HCl (120 mm)
9
10
11
12
13
14
15
16
17
18
HBr (140 mm)
2700
2680
2660
2640
2620
2600
WAVENUMBER (cm⁻¹)

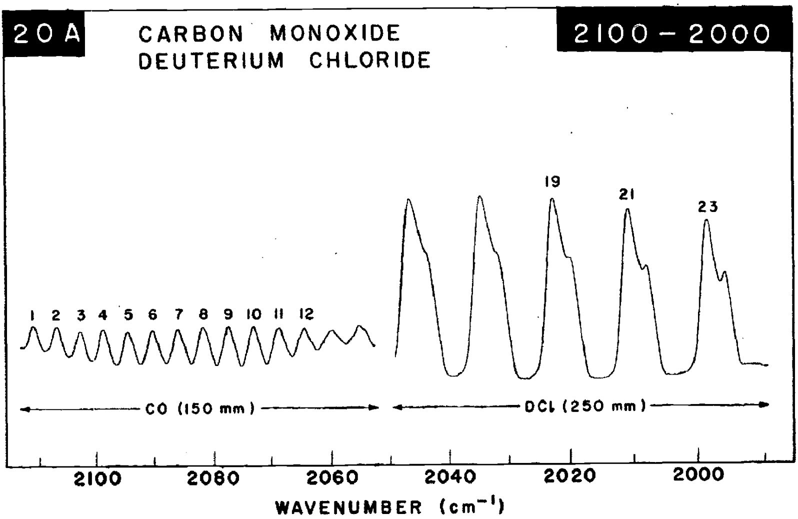

15 A
HYDROGEN BROMIDE
2600 - 2500
1
2
3
4
5
6
HBr (140 mm)
2600
2580
2560
2540
2520
2500
WAVENUMBER (cm⁻¹)

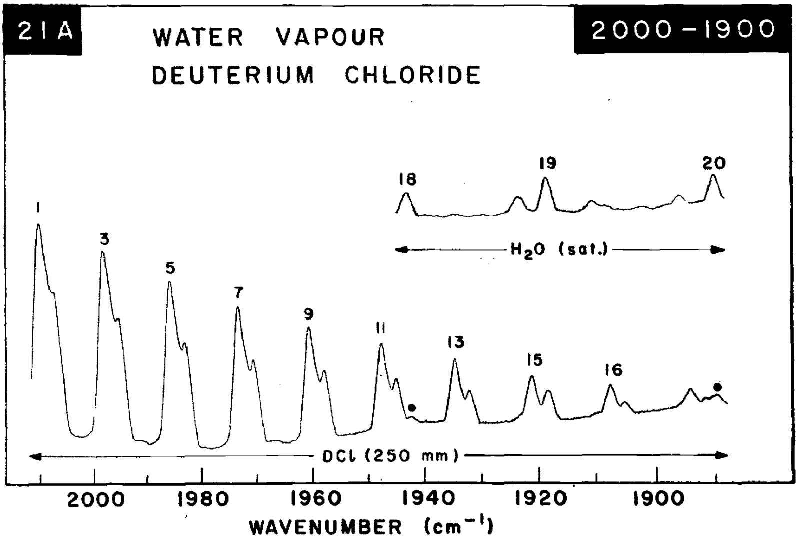

16 A
2500 – 2400
HYDROGEN BROMIDE
1
2
3
4
5
6
7
HBr (140 mm)
2500
2480
2460
2440
2420
2400
WAVENUMBER (cm⁻¹)

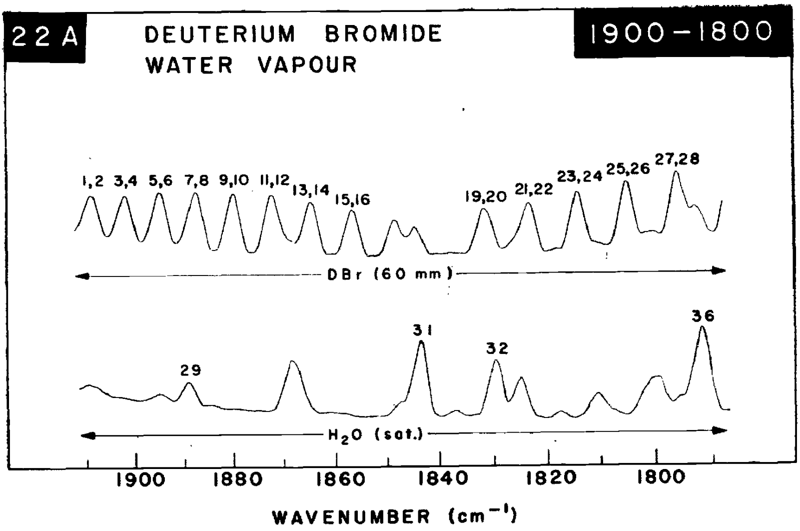

17 A
HYDROGEN BROMIDE
CARBON DIOXIDE
2400 – 2300
1
39
42
44
46
48
50
52
54
56
58
60
HBr (140 mm)
CO₂ (20 mm)
2400
2380
2360
2340
2320
2300
WAVENUMBER (cm⁻¹)

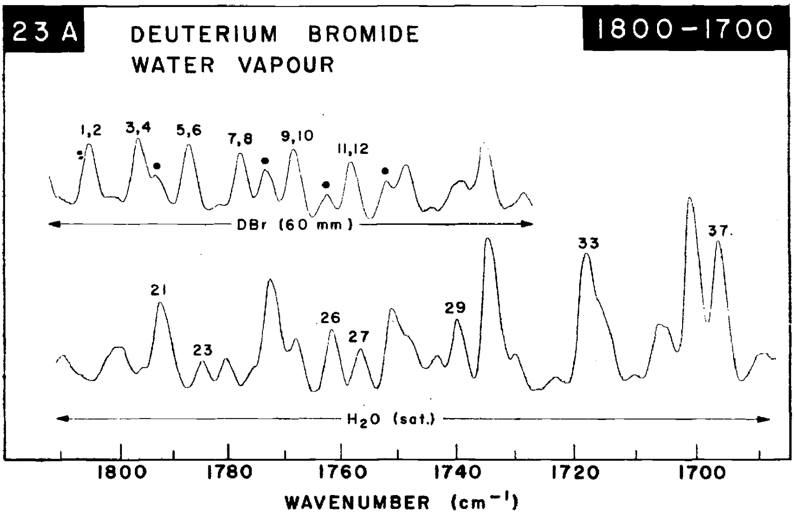

18 A
CARBON DIOXIDE
CARBON MONOXIDE
2300 – 2200
1
2
3
5
7
10
14
16
18
20
22
24
26
28
30
32
37
39
41
43
45
47
49
CO₂ (50 mm)
CO₂ (250 mm)
CO (150 mm)
2300
2280
2260
2240
2220
2200
WAVENUMBER (cm⁻¹)

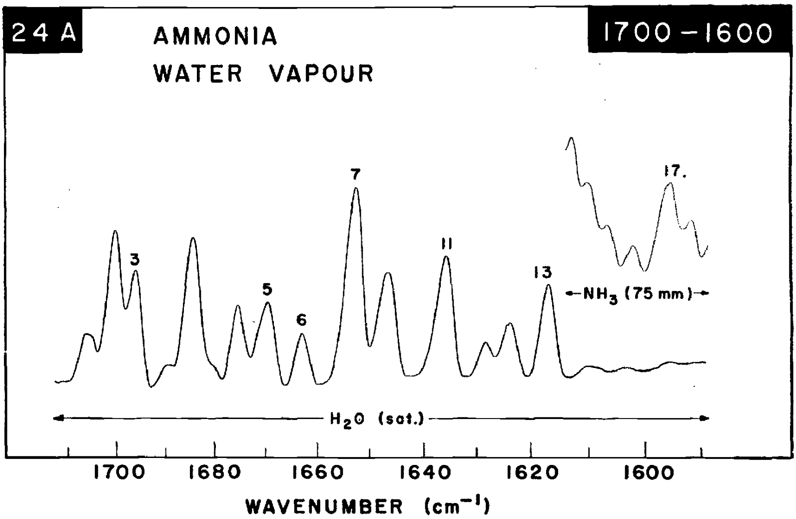

19 A
CARBON MONOXIDE
2200 – 2100
1 3 5 7 9 11 13 15 17 19 20 22 24 26 28 30 32
CO (150 mm)
2200
2180
2160
2140
2120
2100
WAVENUMBER (cm⁻¹)

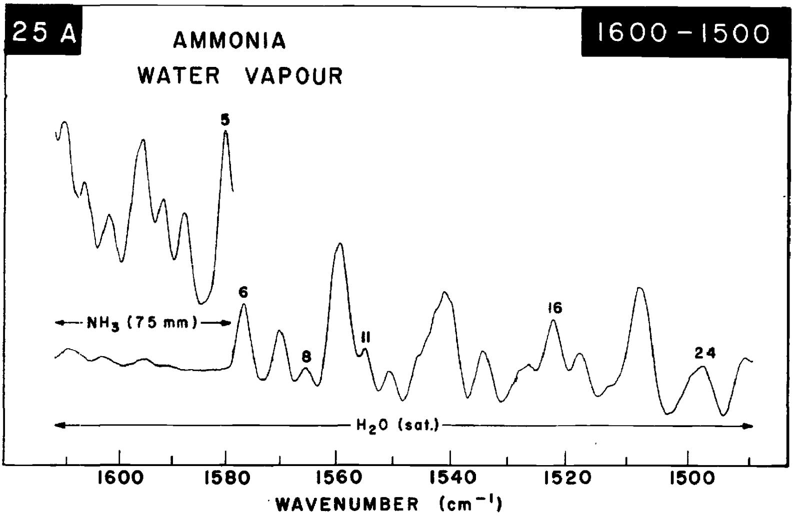

20 A
CARBON MONOXIDE
DEUTERIUM CHLORIDE
2100 – 2000
1 2 3 4 5 6 7 8 9 10 11 12
19 21 23
CO (150 mm)
DCl (250 mm)
2100
2080
2060
2040
2020
2000
WAVENUMBER (cm⁻¹)

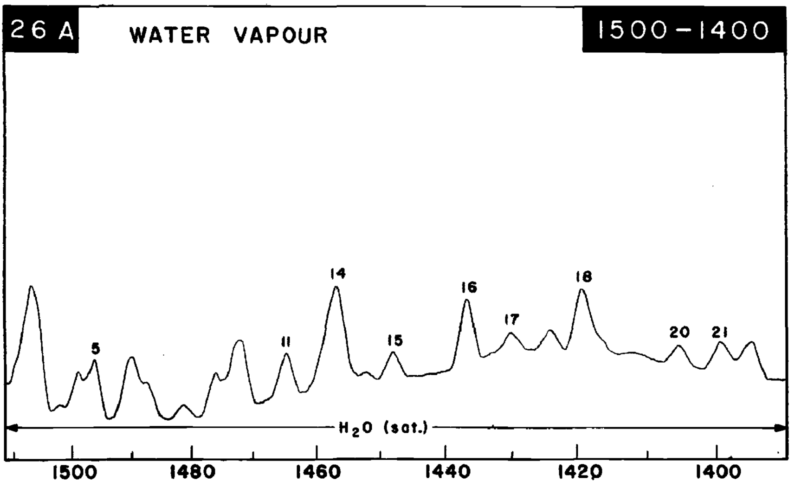

21 A
WATER VAPOUR
DEUTERIUM CHLORIDE
2000 – 1900
18 19 20
H₂O (sat.)
1 3 5 7 9 11 13 15 16
DCl (250 mm)
2000
1980
1960
1940
1920
1900
WAVENUMBER (cm⁻¹)

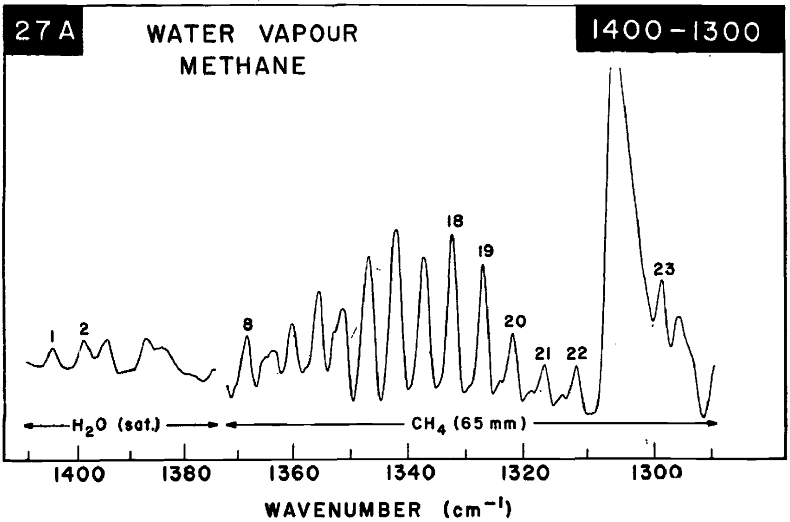

22 A
DEUTERIUM BROMIDE
WATER VAPOUR
1900 – 1800
1,2
3,4
5,6
7,8
9,10
11,12
13,14
15,16
19,20
21,22
23,24
25,26
27,28
DBr (60 mm)
29
31
32
36
H₂O (sat.)
1900
1880
1860
1840
1820
1800
WAVENUMBER (cm⁻¹)

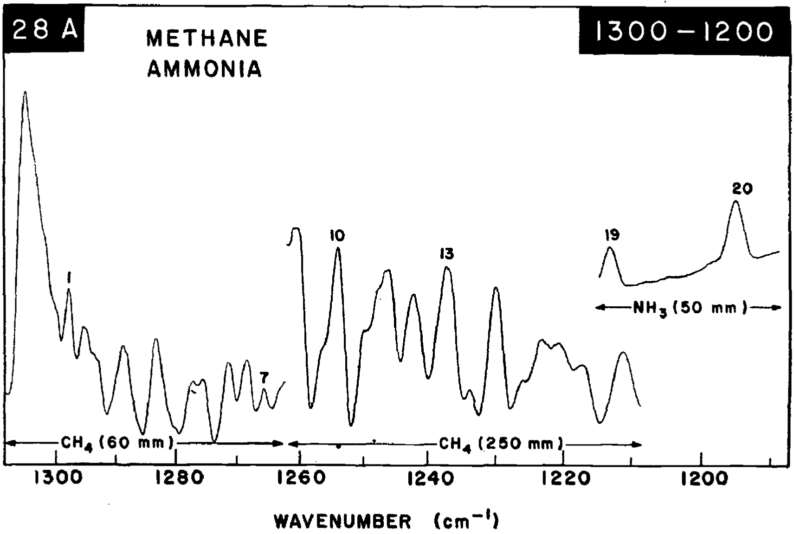

23 A
DEUTERIUM BROMIDE
WATER VAPOUR
1800 – 1700
1,2
3,4
5,6
7,8
9,10
11,12
DBr (60 mm)
21
23
26
27
29
33
37.
H₂O (sat.)
1800
1780
1760
1740
1720
1700
WAVENUMBER (cm⁻¹)

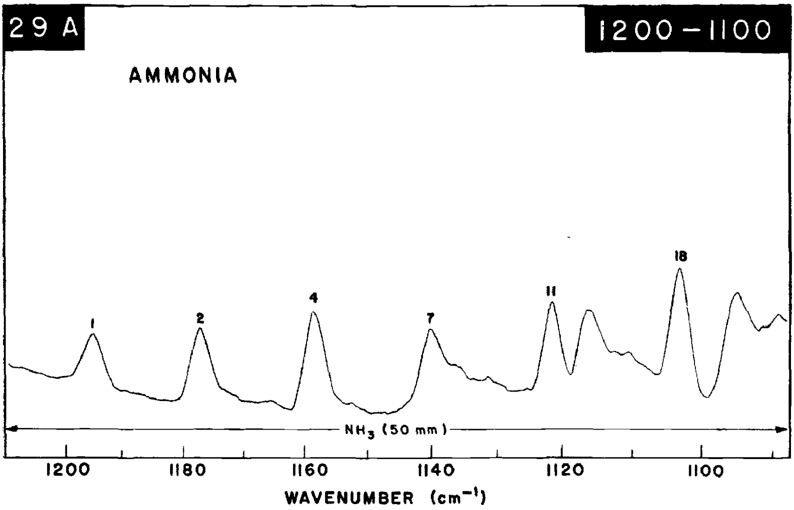

24 A
AMMONIA
WATER VAPOUR
1700 – 1600
3
5
6
7
11
13
17.
NH₃ (75 mm)
H₂O (sat.)
1700
1680
1660
1640
1620
1600
WAVENUMBER (cm⁻¹)

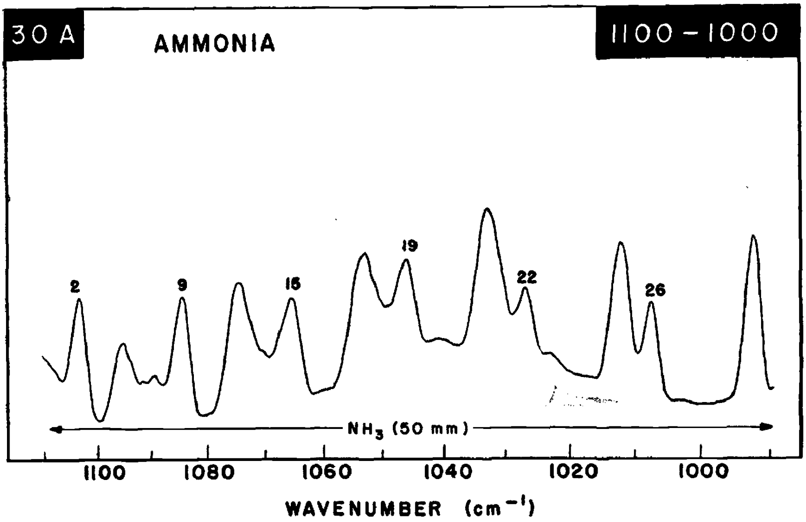

25 A
AMMONIA
WATER VAPOUR
1600 – 1500
5
6
8
11
16
24
NH$_3$ (75 mm)
H$_2$O (sat.)
1600
1580
1560
1540
1520
1500
WAVENUMBER (cm^{-1})

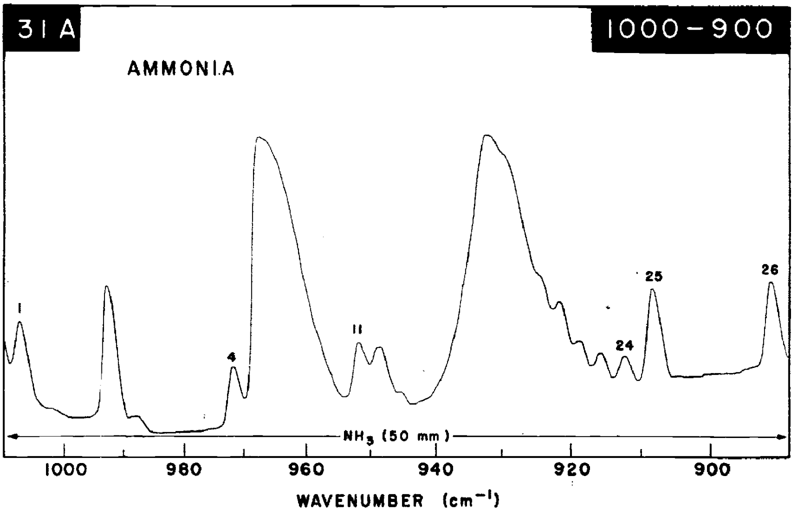

26 A
WATER VAPOUR
1500 – 1400
5
11
14
15
16
17
18
20
21
H$_2$O (sat.)
1500
1480
1460
1440
1420
1400
WAVENUMBER (cm^{-1})

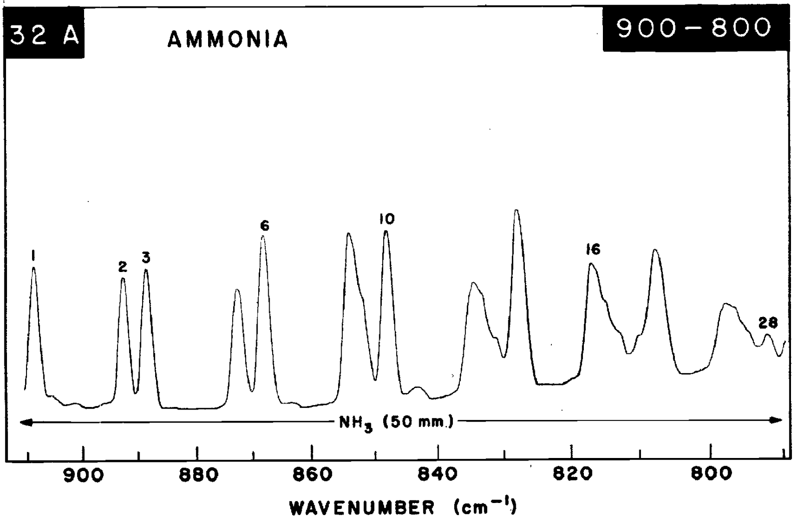

27 A
WATER VAPOUR
METHANE
1400 – 1300
1
2
8
18
19
20
21
22
23
H$_2$O (sat.)
CH$_4$ (65 mm)
1400
1380
1360
1340
1320
1300
WAVENUMBER (cm^{-1})

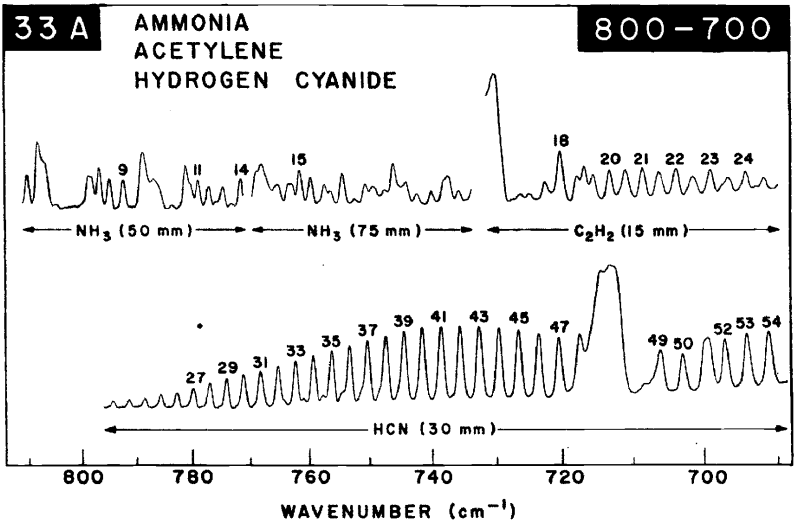

28 A
METHANE
AMMONIA
1300 – 1200
1
7
10
13
19
20
NH₃ (50 mm)
CH₄ (60 mm)
CH₄ (250 mm)
1300
1280
1260
1240
1220
1200
WAVENUMBER (cm⁻¹)

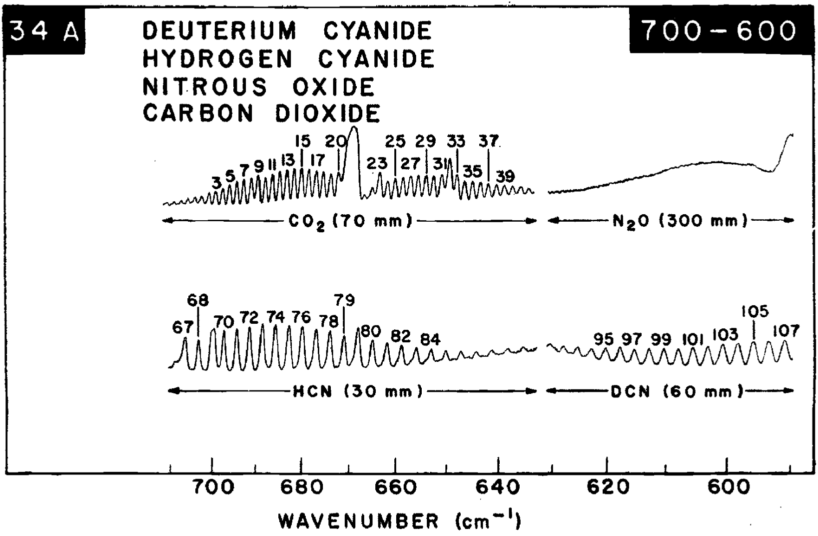

29 A
1200 – 1100
AMMONIA
1
2
4
7
11
18
NH₃ (50 mm)
1200
1180
1160
1140
1120
1100
WAVENUMBER (cm⁻¹)


30 A
AMMONIA
1100 – 1000
2
9
15
19
22
26
NH₃ (50 mm)
1100
1080
1060
1040
1020
1000
WAVENUMBER (cm⁻¹)


31 A
1000 – 900
AMMONIA
1
4
11
24
25
26
NH$_3$ (50 mm)
1000
980
960
940
920
900
WAVENUMBER (cm^{-1})


32 A
AMMONIA
900 – 800
1
2
3
6
10
16
28
NH$_3$ (50 mm.)
900
880
860
840
820
800
WAVENUMBER (cm^{-1})


33 A
AMMONIA
ACETYLENE
HYDROGEN CYANIDE
800 – 700
9
11
14
15
18
20 21 22 23 24
NH$_3$ (50 mm)
NH$_3$ (75 mm)
C$_2$H$_2$ (15 mm)
27 29 31 33 35 37 39 41 43 45 47
49 50 52 53 54
HCN (30 mm)
800
780
760
740
720
700
WAVENUMBER (cm^{-1})


34 A
DEUTERIUM CYANIDE
HYDROGEN CYANIDE
NITROUS OXIDE
CARBON DIOXIDE
700 – 600
3 5 7 9 11 13 15 17 20
23 25 27 29 31 33 35 37 39
CO$_2$ (70 mm)
N$_2$O (300 mm)
67 68 70 72 74 76 78 79 80 82 84
HCN (30 mm)
95 97 99 101 103 105 107
DCN (60 mm)
700
680
660
640
620
600
WAVENUMBER (cm^{-1})