

THE IDENTIFICATION OF MOLECULAR SPECTRA

THIRD EDITION

R.W.B. PEARSE

A.G. GAYDON

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THE IDENTIFICATION OF MOLECULAR SPECTRA

By

R. W. B. PEARSE

D.Sc., F.R.A.S.

*Reader in Spectroscopy,
Imperial College, London*

and

A. G. GAYDON

D.Sc., F.R.S.

*Professor of Molecular Spectroscopy
in the University of London,
Warren Research Fellow of the Royal Society,
Imperial College, London*

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PREFACE TO THIRD EDITION

DURING THE twelve years which have elapsed since the completion of the second edition of these tables many fields of research have found a new interest in spectroscopy. One result of this has been a greater output of papers recording observations of molecular spectra. For this reason an even greater amount of additional material has been added for this edition than for the second. We have endeavoured to include new data up to the end of 1961. To prevent the resulting volume becoming unwieldy we have, as far as possible, presented tables in a more compact form.

The new material takes three forms. First, there are 84 molecules which appear for the first time, observation of their spectra being new; second, there are 135 molecules for which observations have been extended either by addition to the information available for known systems, by the discovery of new systems or by a revision of the previous interpretation of the spectrum; third, the table of persistent heads has been revised and increased by the addition of about 350 new entries.

R. W. B. P.

A. G. G.

IMPERIAL COLLEGE,
LONDON, S.W.7.
APRIL 1962.

PREFACE TO FIRST EDITION

THESE TABLES have been constructed with the aim of facilitating the identification of molecular spectra. Several excellent books have been written dealing with the theory of molecular spectra and some have included collections of molecular constants derived from the analysis of such spectra, yet it has hitherto remained necessary to search through original papers or to calculate the positions of bands from the tables of derived constants in order to identify a given system of bands. This task is usually tedious and sometimes impossible to one without considerable experience.

Originally we prepared for use in the laboratory a list of the wave-lengths of the heads of a limited number of band systems which we frequently encountered as impurities in the course of spectroscopic research. This has proved so useful that it seems worth while to extend the list to cover, as far as possible, all known band systems. Since it appears, moreover, that such a list can be of service, not only to pure spectroscopists, but also to those who use spectroscopy as a tool for research in other fields such as astrophysics, chemistry and chemical technology, we have ventured to gather together in book form such information about known band spectra as may assist in their identification.

In the first list the bands were given in order of wave-length; all bands of the systems considered being included. This arrangement was soon found to possess practical disadvantages. A more useful arrangement was obtained by dividing the data into two sections. The advantages of the division are discussed in the introduction preceding the tables.

As a first stage in the compilation of the available data we have been obliged to limit the scope of the tables in several directions. Thus there are limits to the range of spectrum considered and to the complexity of the molecules whose spectra are included. The wave-length region considered is from 10,000 Å to 2,000 Å, that is roughly from the photographic infra-red to the ultra-violet limit of quartz spectrographs, except that in a few cases, where the origin of a system lies near the border line, one or two bands have been included which are just outside this range. As to complexity we have endeavoured to include all recorded systems of diatomic molecules, but only those of triatomic and more complex molecules which show well-defined banded structure and are of frequent occurrence in spectroscopic investigations. The absorption spectra of complex organic molecules and of solutions have been omitted.

In addition to the wave-lengths of the band heads, the tables include information about the appearance and occurrence of each band spectrum. Though the information thus given is often useful for reference for other purposes, the object of identification has been kept foremost throughout in making decisions relating to the selection and arrangement of material.

For some systems we have found that the existing data are very incomplete. Where these systems are of frequent occurrence we have made new wave-length measurements. In a large number of cases where no estimates of intensities are given in the original paper, but a photograph is included, we have included estimates of intensities made from the photograph. In other cases where the analysis alone is given without mention of the positions and intensities of the most prominent heads, we have located the positions of the heads from the analysis where possible, and if necessary converted the corresponding wave-numbers to wave-lengths. In this connection we should like to point out that it would be of great assistance for purposes of identification if authors of papers reporting new band systems would always in future include a

brief description of the appearance of the system with wave-lengths and intensities of the strongest heads, a few notes on the sources with which it is obtained, and, if possible, publish a photograph with a wave-length scale or a comparison spectrum.

In addition to photographs which we have taken ourselves, we have been very fortunate in having access to numerous spectrograms taken by Professor A. Fowler and his colleagues and students in the Astrophysics Department of the Royal College of Science. Several of the reproductions of common band spectra have been taken from these plates.

Finally, it is with pleasure that we acknowledge our indebtedness to the late Professor A. Fowler for a thorough introduction to the study of spectroscopy and for turning our attention to many of the spectra dealt with herein; to Professor H. Dingle for interest and encouragement in the preparation of these tables; to Dr. W. Jevons, Dr. R. W. Lunt, Dr. E. C. W. Smith, Mr. R. F. Barrow and Mr. R. C. Pankhurst for the use of spectrograms and unpublished data as well as for useful criticism during trial of the tables, and to Mr. E. S. Parke for very valuable assistance in the preparation of the plates. One of us (A. G. G.) is also indebted to the Trustees of the Beit Fellowships for Scientific Research for a special grant, during the tenure of which a large part of the manuscript was compiled.

R. W. B. P.
A. G. G.

LONDON.
SEPTEMBER 1940.

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INTRODUCTION

EXPERIENCE in using the list of band heads arranged in order of wave-length showed that in extending it to include many more molecules a modification of form was desirable. The Tables for the Identification of Molecular Spectra are therefore divided into two sections.

The first section consists of a list of the strongest heads of the more persistent and better known band systems of each molecule in order of wave-length, together with information as to origin, intensity in various sources, and appearance.

The second section consists of individual lists of band heads for each system of each molecule, accompanied by notes about the occurrence and appearance of the system, the nature of the electronic transition involved, the vibrational assignment of the bands in the system, and references to the sources of the data. The lists are arranged in alphabetical order of the chemical symbols of the molecules.

The general considerations leading to this division are briefly as follows. For practical reasons it is preferable to identify the molecular contribution to a given spectrum, system by system, rather than band by band. It is the practice to identify the atomic contribution, line by line, with the aid of tables of atomic lines in order of wave-length and there is a natural tendency to proceed to identify bands in a similar way. Such a procedure, however, frequently leads to incorrect identification. In an atom each change of electronic state gives rise to a line, whereas in a molecule each change of electronic state gives rise to a band system. The various bands of the system arise from changes of the vibrational state of the molecule and in general involve much smaller energy intervals than the electronic changes. Thus in respect of variation of intensity from source to source the bands of one system behave somewhat like the components of a fairly close multiplet, appearing and disappearing together. But whereas the multiplet contains relatively few lines of the whole spectrum, a single band system often contains several hundred bands and may comprise all the radiation that is readily excited for that particular molecule. Inclusion of all such bands in a single list leads to a large number of coincidences in wave-length which are merely fortuitous. Such coincidences are more troublesome in the case of bands than in the case of lines, since the wave-length recorded for a band head depends very considerably on the judgment of the observer and the dispersion used. This makes it much less safe to identify a single band by wave-length alone than it does to identify a single line in this way. Supporting evidence should always be sought. Such evidence can be obtained by considering the system as a whole. The list of Section I has therefore been restricted to a few of the strongest bands of each system so that it is somewhat analogous to the list of persistent lines of the elements. The actual number and choice of bands which should be included in this list is mainly a matter for experience to decide. The purpose of the list is to provide a clue to the identity of an unrecognised system. The strongest band of the unknown system is compared with the list, and a close agreement of wave-length and direction of degradation may suggest that it is a member of a certain system of a given molecule. Reference is then made to the individual

list for that system and the presence or absence of other members checked. The process is then continued with the strongest of the remaining unidentified bands, and so on. It is also advisable to look for other systems of the molecules for which systems are found as well as for systems of other molecules containing the same elements. Thus if a system of C_2 is found and a system of N_2 , it is well to look for systems of CN as well as for other systems of N_2 and C_2 . Or, again, if a trace of oxygen is suspected, systems of NO and CO may be looked for. This procedure often leads to the discovery of weak bands, masked by stronger bands, which would otherwise have passed unnoticed. In following up other systems in this manner, and indeed in all cases where interest lies in the spectrum of a given molecule, the arrangement of Section II is especially convenient. It is well also to emphasise that the evidence of atomic lines should not be neglected.

To facilitate the checking of the presence of atoms a table of persistent lines of the elements has been included in the appendix. If it is desired to check the line spectra more fully, recourse should be had to the various tables of atomic lines that are available.

Finally, in as much as direct comparison of photographs is the quickest and most certain way to identification, a number of plates are included showing many of the more frequently encountered band systems.

TABLE OF PERSISTENT BAND HEADS

THE OBJECT OF THIS TABLE is to provide a clue to the nature of the unknown band system as quickly as possible, so that it may be compared directly with the appropriate detailed list. For this purpose it contains, for all suitable band systems of frequent occurrence, a selection of the outstanding heads, which are most conspicuous under various conditions of excitation, arranged in order of wave-length. The actual number of bands of a system included is somewhat arbitrary, and the optimum can only be decided by extensive trial of the list. The general considerations are that there should be sufficient bands to provide a clue, whether the system is observed in emission or absorption, but not so many as to multiply unduly the possibility of chance coincidences. In a great number of cases, when the band system is composed of well-marked sequences, the requirements are well fulfilled by giving the first heads of the (1, 0), (0, 0) and (0, 1) bands. In other cases, however, where the molecular constants differ greatly for the two electronic states involved, the strongest bands are often far from the system origin and, moreover, those which are conspicuous in emission are weak in absorption, and *vice versa*. The Schumann-Runge bands of O_2 may be quoted as an extreme example of this behaviour. Then, again, the nature of the overlapping background of band structure decides to a considerable extent how conspicuous is a given head. Thus, the first head of a sequence is usually more outstanding than a slightly stronger head further along the sequence, on account of greater contrast with the background, and so is given preference. Similarly, in the case of close double or triple heads, it is usually the first head which is included in the list. In difficult systems the best selection can only be made from a series of photographs taken under various conditions. However, even if the absence of such photographs has in a few cases caused the omission of the *most* conspicuous head, nevertheless the heads included should be among the outstanding ones, so that by trial of two or three heads from the unknown spectrum a coincidence should be obtained.

Wave-lengths. In the first column are given the wave-lengths in air in International Angstroms, values being quoted, where possible, to the nearest 0.1 Å. Bands which are of particularly frequent occurrence as impurities are marked by an asterisk* before the wave-length. The letter R, V or M immediately following the wave-length indicates that the measurement is for the head of a band degraded to longer (red), shorter (violet) wave-lengths or is the maximum of a headless band respectively. The letter O is used in a few cases to signify that the wave-length recorded refers to the origin of the band.

Intensities. Intensities are eye estimates based on a scale of 10 for the strongest band of the system (or in a few cases for the strongest band of all the systems of that particular molecule), and they therefore usually refer only to the relative intensities of the bands within the system. Intensities printed in ordinary type are derived from actual experimental observations on the given source. Intensities given in italics are

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estimates based on consideration of the vibrational distribution of intensity in other sources and imply that the band has been observed in the given source, but the observer has omitted to record intensities. Absence of a figure for intensity in any particular column merely indicates that the authors have no knowledge of the occurrence of the system in that source, but a dash, —, denotes that under normal experimental conditions the band is unlikely to occur in that source (*e.g.*, a band arising from a transition between the two excited electronic states will not in general be observed in absorption at ordinary temperatures).

Sources. Intensities are listed for the following sources:

Ab.	Absorption in vapour state.
F.	Emission in flame.
A(a).	Emission in an arc at atmospheric pressure, usually in air.
A(r).	In an arc at reduced pressure (frequently referred to as a vacuum arc). Bands occurring in arc sources are listed under only one of these (a) or (r), that which is more favourable to the band.
D+ } D- }	In discharge tubes of various sorts. The + and - columns denote whether the band appears more readily in the positive column or the negative glow respectively. Bands occurring in special discharges such as a high-frequency electrodeless discharge are usually listed in the positive column with an additional note under "Occ."

Appearance. Some indication of the appearance of the band is given in the last column but one, the following abbreviations being used:

CD.	Close double head (separation $\frac{1}{4}$ –2 Å).
CT.	Close triple head (separation $\frac{1}{4}$ –2 Å).
D.	Double head (separation 2–15 Å).
DCD.	Double head, each component a close double.
F.	Group of four or five heads.
Fd.	Group of five heads appearing double with small dispersion.
L.	Narrow band resembling an atomic line.
S.	Head of a sequence or group of bands.
T.	Triple head (separation 2–15 Å).
wr.	Accompanied by weaker head to the red.
wv.	Accompanied by weaker head to the violet.

Occurrence. In the last column headed "Occ." some indications are given of special conditions or sources which are particularly favourable to the production of the band, the following abbreviations being used:

c.	Mildly condensed discharge.
e.	Controlled electron source.
f.	Fluorescence.
fp.	Absorption following flash photolysis.
hc.	Hollow cathode of discharge tube.
hf.	Electrodeless high-frequency discharge.
Kf.	Emission or absorption in King furnace.
r.	Ring discharge.
sw.	Shock wave (<i>i.e.</i> emission in shock tube).

t.	Tesla coil.
A.	Favoured by presence of argon.
H.	„ „ hydrogen
He.	„ „ helium.
N.	Excited by active nitrogen.
Ne.	Favoured by presence of neon.

Very Extensive Systems. Some systems comprise a very large number of bands which differ little in intensity and cover a wide range of the spectrum. Because of the large number of bands which would have to be included for identification in the list of persistent heads they have in many cases been omitted. The extensive character of these systems in itself provides a clue to their identity.

The following is a list of the most important molecules which emit such extensive systems with the approximate region of the spectrum covered. Unless stated to the contrary, all these systems consist of bands degraded to longer wave-lengths (red).

As ₂	4300-2250 Å	Li ₂	7700-6600, 5000-4700.
Br ₂	> 8000-5100.	LiH	5000-3000.
CO flame (narrow headless)	6000-3000.	Na ₂	7000-6000, 5100-4800, 3500-2500.
Cl ₂	> 6000-4800.	NaH	5000-3700.
CsH	6500-5000.	NaK	9100-7200, 6000-5700, 5300-4900, 4000-3800.
H ₂	"many-line."	P ₂	3300-2000.
I ₂	> 8000-5000.	Rb ₂	7100-6700, 5200-4500.
IBr	> 7000-5500.	RbH	6500-5000.
ICl	> 8000-5700.	Se ₂	3700-3000.
K ₂	8900-7700, 7000-6200, 4500-4200.	Te ₂	4900-3900.
KH	5500-4000.		

The following molecules show extensive systems which are partly included in the table of persistent heads:

CN	"Cyanogen red," 9400-4700.
CO	"Fourth Positive," 2800-< 2000.
N ₂	"First Positive," > 10,000-5000.
O ₂	"Schumann-Runge emission," 4400-< 2200.
O ₂ ⁺	"Second Negative," 6000-2000.
S ₂	6000-2800.
SO ₂	absorption 3400-2500.
SiF	6500-2500 (bands degraded both ways).
SiO	3000-< 2000.

	Ab.	F.	A(a).	A(r).	D ⁺ .	D ⁻ .	System.	App.	Occ.
10828 R			10				BeO	Red	
10803.3 R				10	10		BaH		
10510.0 V	—	—			10		N ₂	1st Positive	T.S.
10052 R				10	10		BaH		
9919.9 R			3				TaO		
9868.6 R			10				TaO		
9849.3 R			6				TaO		
*9834.7 V			10				CaO		S.
9669 R		7					H ₂ O		
9647.5 R			8				BeO	Red	

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	Ab.	F.	A(a).	A(r).	D ⁺ .	D ⁻ .	System.	App.	Occ.
9420 O	9						H ₂ O		
9329.9 R			10				ZrO		
9315.9 R			10				ZrO		
9299.6 R			10				ZrO		
9277 R		10					H ₂ O		
*9229 R			10				CaO	S.	
9197.4 R			3				TaO		
9195.8 R			?				SrO		
9152 R	5	5					HCl		
*9148.3 R		7			7		CN	Cyanogen Red	T.wv. N.
9098 R		10					BaCl		
9060 O	6						H ₂ O		
9017 R				10	10		BaH		
8924 R				10	10		BaH		
8916 R		7					H ₂ O		
8912.4 R	—	—			10		N ₂	1st Positive	T.S.
8859.6 R			10				TiO	S.D.	
8829.4 R		10					OH	Meinel	D. H+O ₃
8752.5 R	10				10		MnCl	S.	hf.
*8722.3 V	—	—			8		N ₂	1st Positive	T.
8700.0 R			?				SrO		
8675 R	—	—			10		N ₂	I-R Afterglow	T.
*8652.2 R			8				CaO	S.	
8624.0 R			7				VO		
8619.8V	—	—			10		NO	I-R Quartet	N.
8611.1 R	10	10					CrH	S	Kf.
8597.8 R		4			4		O ₃	Atmospheric	
8571.5 R		7	7				BaF	S.	
8537.7 R			7				VO		
8563 O	5						HCN		
*8541.8 V	—	—			6		N ₂	1st Positive	T.
8420.8 R		10					BaCl		
*8406.0 R			1				LaO	S.	
8297 R		8	8				FeO		
8293.4 R.	—	—				5	N ₂ ⁺	Meinel	T. He.
8282.7 R	10	10					BiO		
8257.8 R			?				SrO		
8238.0 V					7		MnF		hf.
8228 R		8	8				FeO		
8227 O	8						H ₂ O		
8192 R			?				ZrO		
*8167.3 R			7				CaO		
*8153.0 R			9				CaO	S.	
8137 R		8	8				FeO		
8137.0 R		7	7				BaF	S.	
8106 R		10	10				FeO		
8097 R		8					H ₂ O		
8057.6 V	—	—			10		N ₂	Herman's I-R	S. t.
8053.6 R	—	—				8	N ₂ ⁺	Meinel	T. He.
7978.4 R					10		BS	DCD	

TABLE OF PERSISTENT BAND HEADS

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	Ab.	F.	A(a).	A(r).	D ⁺ .	D ⁻ .	System.	App.	Occ.
7952 R			10				BeO		
7919 M	9						NH ₃		
7918.5 R		8					OH	Meinel	H+O ₂
7912 O	8						HCN		
*7910.5 R			8				LaO		
7896.0 R			10				VO		
7879.3 R			10				CeO		
*7877.2 R			6				LaO	S.	
*7876.4 R		10			10		CN	Cyanogen Red	T.wv N.
7865.0 R			9				VO		
7861.9 V	—	—			5		NO	I-R Quartet	N.
7852.5 V	—	—			3		C ₂	High Pressure	D. c.
7850.9 R			6				VO		
7845 R		10	10				BiO		
7833.9 R	—	—			3		CO	Asundi	T.
7831.8 R			10				CeO	S.	
7828.0 R			8				TiO	γ	
7825.7 R	—	—				10	N ₂ ⁺	Meinel	T. He.
7787.6 V	—	—			5		NO	I-R Quartet	N.
7780 R	—	—			10		N ₂	I-R Afterglow	T.
7755.8 R		10					OH	Meinel	H+O ₂
*7753.2 V	—	—			6		N ₂	1st Positive	T.S.
7743.2 R			10				WO		
*7715.5 R			8				CaO		
*7687.8 R			8				CaO		
7672.1 R			8				TiO	γ	
7628.1 R			7				TiO	γ	
*7626.2 V	—	—			7		N ₂	1st Positive	T.
7593.7 R	10	10			10		O ₂	Atmospheric	
7591 R	—	—			10		N ₂	I-R Afterglow	T.
7589.6 R			7				TiO	γ	
7529.1 R		3					OH	Meinel	H+O ₂
7521.0 V	—	—			4		N ₂	Herman's I-R	S. t.
7508 V				10	10		SrH		
*7503.9 V	—	—			7		N ₂	1st Positive	T.
7463 R	3	3					HCl		
*7403.5 R			10				LaO		
*7386.6 V	—	—			5		N ₂	1st Positive	T.
*7379.8 R			8				LaO	S.	
7379.3 R	10						HND	F.	fp.
7350 V	10	10					NH ₃		fp.
7348.0 V				10	10		SrH		
7346.7 V				10	10		γ		
7333.8 R			5				VO		
*7318.5 R			7				CaO		
7311.7 R					10		BS	DCD.	
*7308.3 R			1				CaO	S.	
7297.2 R			10				CeO	S.	
7284.2 R		5					OH	Meinel	H+O ₂
7277.3 R	10	10					BiO		

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	Ab.	F.	A(s).	A(r).	D ⁺ .	D ⁻ .	System.	App.	Occ.
7275.5 R			10				CoO		
7245.9 V						10	AlF	S.	
7235.8 R			10				CoO	S.	
7227 O	5						H ₂ O		
7210.4 R	—	—			5		CO	Asundi	T.
7197.7 R			7				TiO	γ	
7164.5 R		6					H ₂ O		
7125.6 R			10				TiO	γ	
7116.0 R	10	8	8				BaF		D.S.
7087.9 R			9				TiO	γ	
7083.2 V	—	—			4		C ₂	High Pressure	D.
7069.8 R			10				WO		c.
7054.5 R			7				TiO	γ	
7036.8 R	—	—				4	N ₂ ⁺	Meinel	T.
7030 R				5			SnH		He. H.
7018.1 V				10	10		SrH		
7011.0 V	10						SrI	S.	
*6994.5 R			1				LaO	S.	
6984.7 V				10	10		SrH		
6942.6 V				10	10		CaH		
6936.5 R		10	10				BiO		
6930.2 V	10						SrI	S.	
6922.0 R		2					H ₂ O		
6896 R	—	—			8		N ₂	I-R Afterglow	T.
6892 R				5			SnH		H.
6890.7 R					10		MnF		S.
6867.2 R	8	2			2		O ₂	Atmospheric	hf.
*6856.3 V	—	—	—			8	O ₂ ⁺	1st Negative	
6853.0 R	—	—				3	N ₂ ⁺	Meinel	T.
6850.2 V				10	10		BaH		He.
6847.7 V	10						SrI		S.
6820 M		8		8			SrOH		
6804.0 R	—	—			8		CO	Asundi	T.
*6788.6 V	—	—			6		N ₂	1st Positive	T.
6782.8 R		8	8				BaO		sw.
6767.8 V	10						SrI		S.
6763.3 R						10	RaCl		S.
6745 R				5			SnH		He. hc. H.
6737.1 R			5				ChO		
6708.8 R		10	10				BiO		
*6704.8 V	—	—			8		N ₂	1st Positive	T.
6689.5 V				10	10		BaH		
6685.7 R	—	—			7		CO	Asundi	T.
6675 M		8		8			SrOH		
6672.4 V			10				—	Sr oxide	
6666.7 V	10	10					SrBr		S.
6655.6 V	7	7	7				SrF		S.
6652 M		5					NH ₃	Ammonia α	
6651.5 R			4				TiO	γ	S.
6632.7 V	10	10	10				SrF		S.

TABLE OF PERSISTENT BAND HEADS

9

	Ab.	F.	A(a).	A(r).	D ⁺ .	D ⁻ .	System.	App.	Occ.
*6631.6 R	—	4	9		9		CN	Cyanogen Red	T. vv.
*6623.6 V	—	—			9		N ₂	1st Positive	T.
6620 M	10	—					NO ₂		
*6620.3 V	—	—			7		CO	Angstrom	
6619.9 V	4	1	5				SrCl		S.
6613.7 V	10	10	10				SrCl		S.
6607.6 R					7		RaCl		S.
6590 M		8		8			SrOH		He. hc.
6569.3 R			7				TiO		
6559.1 R			9				SbO		
6550.0 R		10					IF		
*6544.8 V	—	—			10		N ₂	1st Positive	T.
6543.0 R			5				ZrO	γ	
6533.5			9				SmO		
6521.4 V			10				—	Sr oxide	
6518.6 R					10		F ₂		
6516.8 M		5					H ₂ O		
6513.5 R	—	—			9		CO	Asundi	T.
6513.0 V	5	10					SrBr		S.
6512.0 V	10	10	10				SrF		S.
6510.9			10				SmO		
6508.1 R			9				ZrO	γ	
6498.1 R					10		RaCl		S.
6494.8 R			5				CbO		He. hc.
6493.4 R			1				CuO		N.
6493.1 R		9	9				BaO		sw.
6492 V					5		SiF	ξ	
6490.4 M		5					H ₂ O		
6481.6 R		10					IF		
*6478.4 R		10			10		CN	Cyanogen Red	T. vv.
6474.1 V					10		FeCl		S.
6473.7 R			10				ZrO	γ	hf.
*6468.5 V	—	—			10		N ₂	1st Positive	T.
6468.0 M		5					H ₂ O		
6464.6 R	—	—			10		CO	Triplet	He. H.
6460 M		8		8			SrOH		
6457 M			10				—	Sr oxide	
6451.5 R		7	7				CrO		sw.
6446.2 R			5				ScO		
6442.3 V	—				6		C ₂	High Pressure	D.
6433.1 R	—	—			10		CO	Triplet	He. H.
6430.0 R			3				CuO		N.
6419.0 V		8	8				SrF		S.
*6418.7 V	—	—	—		9		O ₂ ⁺	1st Negative	
6416 V					5		SiF	ξ	
6412.9 V	10	7					CaI		S. wr.
6412.3 R			6				ZrO	γ	
6407 R	6	10					BrF		
6400.4 R		1	5				CuO		N.
6399.0 R	—	—			10		CO	Triplet	CD.