THE IDENTIFICATION OF MOLECULAR SPECTRA

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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 wavelengths 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 wavelength; 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 wavelength region considered is from 10 000 Å to 2000 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 the 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 wavelengths 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 wavelength 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 wavelengths. 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 wavelengths 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 wavelength 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, Dr. R. F. Barrow and Dr. 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.

Preface to Fourth Edition

The first edition of this book appeared in 1941, the second in 1950, the third in 1963, and, as this sold out quickly, we had it reprinted with a 20-page supplement in 1965. This edition has been very fully revised. The first edition contained information about spectra of around 250 diatomic molecules and 35 polyatomic; this one covers about 490 diatomic and 127 polyatomic. Developments in techniques, such as flash photolysis, and interest in new subjects such as upper-atmosphere chemistry have contributed to the expansion of the amount of data available.

We have done our best to comb the literature up to about the end of 1974. Data listed are based on original papers or, in some cases, on our own measurements, but the compilations edited by B. Rosen *et al.* (*Données Spectroscopiques Relatives aux Molécules Diatomiques, 1970*) and its supplement edited by R. F. Barrow *et al.* (*Diatomic Molecules; A Critical Bibliography of Spectroscopic Data*, 1973), the book by G. Herzberg (*Electronic Spectra of Polyatomic Molecules*, Van Nostrand, 1966) and the Berkeley Newsletters on *Analysis of Molecular Spectra*, prepared regularly by J. G. Phillips and S. P. Davis have been of great value in tracing references to the literature.

Although other works, such as that edited by Rosen, give constants and some data for diatomic molecules, and the book by Herzberg gives molecular constants for polyatomic molecules, this is still the only work aimed primarily at Identification, giving both diatomic and polyatomic molecules and including a considerable collection of reproductions of the actual spectra.

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

LONDON.
AUGUST 1975.

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Introduction

Experience in using the first list which we drew up of band heads arranged in order of wavelength, showed that in extending this list to include a large number of molecules it was desirable to modify the system. The Tables for the Identification of Molecular Spectra are therefore divided into two sections.

The first section consists of a list of the most prominent heads of the more persistent and better-known band systems of each molecule. These heads are listed in order of wavelength, with abbreviated information about the direction of degradation of the bands and their appearance, and, of course, the molecule responsible. In earlier editions we made an attempt to include estimates of relative intensity of the heads within the system, listing these intensities under the sources in which the head was likely to be observed; however, since only the most prominent heads of each system were included, most of the intensities were '10' and in many cases information was not really adequate. This information about intensities has therefore been omitted from the first section in this Fourth Edition. This has enabled the table to be set more compactly.

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 of the system, intensity estimates on a visual scale and references to the source 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 wavelength and there is a natural tendency to proceed to identify bands in a similar way. Such a procedure, however, often leads to incorrect identification. In an atom, each change of electronic state gives rise to a line, whereas in a molecule each change in electronic state gives rise to a whole band system. The various bands within the system arise from changes of the vibrational energy 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 many heads, perhaps several hundreds, 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 chance coincidences in wavelength. Such coincidences are more troublesome in the case of bands than in the case of lines, since the wavelength recorded for a band head is seldom as precise as that for an atomic line, depending, because of the structure of the head itself, very considerably on the judgement of the observer and on the dispersion used. This makes it much less safe to identify a single band by wavelength alone than it does to identify a single atomic 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 most prominent heads of each system so that it is somewhat analogous to the list of persistent lines of the elements. The purpose of the list is to provide a clue to the identity of an unrecognised system. The most prominent head of the unknown system is selected. This will usually be the front head of the strongest band, but not necessarily the strongest individual head for a multi-headed band. This head is then compared with the Persistent Heads list and a close agreement of wavelength 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 is checked. The process is then continued with outstanding heads of 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 and also for systems of other molecules containing the same elements; thus if a system of C_2 is found and also one of N_2, it is desirable to look for systems of CN as well as others systems of C_2 and N_2. Or, again, if a trace of oxygen is suspected, systems of NO and CO may be checked. This procedure often leads to the discovery of weak bands, masked by stronger ones, 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.

The actual number and choice of bands which should be included in the two lists is mainly a matter for experience to decide. We have tried to place most emphasis on those molecules which are cosmically abundant or are known to occur readily as impurities. Since the first edition of the book a very large number of new molecular spectra have been reported. In some cases this may almost degenerate to 'stamp collecting'; studies of rare molecules involving unusual combinations of elements form convenient Ph.D. projects for students. However, it is often very difficult to predict what will and what will not be useful. For example the prominence of ZrO bands in some stellar spectra could hardly have been foreseen. Unusual molecules may arise from use of rare elements in transistor materials; development of special laser system may require unusual species; pollution by toxic heavy metals, like cadmium, may involve unusual spectra in their estimation. For common molecules we have tended to give the prominent bands of all known systems; for the rarer species we have usually included only the strongest band or two of the strongest system in the first list of Persistent Heads, and to give all systems but only a few bands of each in the second list, Individual Systems. Some band systems are very extensive, involving many bands of comparable intensity. These present special difficulty and it is not possible readily to identify such systems from the main Persistent Heads table.

It is well to emphasise that in making identifications, the evidence of the presence of atomic lines may be very helpful. 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 made 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 of identification, a number of plates are included showing many of the more frequently encountered band systems. Also those references to papers which contain a useful reproduction of the spectrum are indicated by a dagger, †, following the date.

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 or with one of the plates. For this purpose the list contains for all suitable band systems which are of frequent occurrence a few (sometimes only one) of the outstanding band heads, arranged in decreasing order of wavelength.

In this fourth edition the structure of this table has been substantially modified because of the large increase in the number of known band systems. For the simplest systems with strong (0, 0) sequence we have included just this one head. In a greater number of cases we have given the heads of the (0, 1), (0, 0) and (1, 0) sequences. For systems with more open Franck-Condon intensity parabolae we have had to include more heads, but have kept the number down to the minimum. To include many heads not only makes the table long and expensive to set but increases the risk of chance meaningless coincidences.

Following the wavelength we have given a brief indication of the appearance of the head. This always includes the direction of degradation

R degraded to longer wavelengths (red)

V degraded to shorter wavelengths (violet)

or that the band measurement is for the maximum, **M**, of a headless band, or is the origin, **O**, of a band with a clear region near the origin and branches spreading in each direction from this origin. **L** indicates a very narrow, line-like, feature.

Other remarks in this appearance column are:

CD. Close double head (separation usually less than 5 Å).

CT. Close triple head.

D. Double head.

DCD. Double head, each component a close double.

F. Group of four or more heads.

L. Narrow band resembling an atomic line.

T. Triple head.

wr. Accompanied by weaker head to the red.

wv. Accompanied by weaker head to shorter wavelengths (violet).

We should stress that we have usually given the *first* or most prominent head of the sequence, not necessarily the strongest. Some molecules have very extensive band systems consisting of many bands of comparable intensity and it has not been possible to include these. It often happens that homonuclear molecules have spectra of this type and examples are As_2, Br_2, Cl_2, I_2, K_2, Li_2, Na_2, P_2, Se_2, Te_2. Some mixed molecules of the same group of the periodic table also tend to give extensive systems, e.g. IBr, ICl, NaK. We have also excluded from this table the very rare molecules, the collector's pieces.

In previous editions we listed intensities, often hypothetical, for the band in each of six sources. However, since we are always selecting just the strongest bands, these intensities were mostly 10 or 9 and not of much help, and since this arrangement took up a lot of space and required a lot of rather arbitrary decisions on our part, we have now dropped the inclusion of intensities from this list of persistent heads.

We have, however, retained the asterisk, *, to denote those bands which in our experience occur rather frequently as impurities in other spectra.

For those molecules of importance possessing a number of strong systems, such as CO, N_2, CN, we have given in very abbreviated form an indication of the system following the symbols for the

molecule, e.g.

N_2 1st Pos. Nitrogen First Positive System

C_2 Desl.-d'A. Deslandres-d'Azambuja's System

In making an identification using this table, the procedure should be to select *several* of the most prominent heads of the unknown system and to compare these with the table. If the wavelength of one of them coincides with that in the table, and the direction of degradation is right, then further comparison should be made with the individual lists. This is just a table of persistent heads, not all heads.

λ	*App.*	*Mol.*	*System*
9874·4	R, T	BaH	
9868·6	R	TaO	
9849·3	R	TaO	
*9835·0	R	CaO	
9589·1	R	RhC	
9776·1	R	SrO	
9725	R, D	TiO	δ
*9669	R	H_2O	
9658·0	R	BaCl	
9647·5	R, D	BeO	
9513·5	R	BaH	
9494	R	SeO	
9400	R	OH	Meinel
9357·2	R, T	BaH	
9299·6	R	ZrO	
*9277	R	H_2O	
9195·8	R	SrO	
9152	R	HCl	
9145·3	R, T	N_2^+	Meinel Aur.
*9140·6	R, T, wv	CN	Red
9123·1	R	He_2	
9101·7	R	BaCl	
9098	R	BaCl	
9062·4	R	TiS	
9026·1	R	BaH	
8981·7	R, D	BaH	
*8980·5	R	C_2	Phillips
8859·6	R, D	TiO	δ
8829·4	R, D	OH	Meinel
8742·4	V, wr	NF	
*8722·3	V, T	N_2	1st Pos.
8700·0	R	SrO	
8685·4	R	NiCl	
8675	R	N_2	I-R Aft.
*8652·2	R	CaO	
8626·0	R, T	TiS	
8624·0	R	VO	
8619·8	V	NO	I-R Quartet
8613·3	R	SO	
8611·1	R	CrH	
*8597·8	R	O_2	Atmosph.
8585·5	V	C_2O	
8571·5	R	BaF	
8557·8	V	C_2O	
*8541·8	V, T	N_2	1st Pos.
8488·9	R	PrO	
8451·2	R	BaH	
8448·1	V	PH_2	
8435·9	O	SiF	
8421·6	R, D	BaH	
8420·8	R	BaCl	
8394·6	R	NiCl	
8283·6	R	TiS	
8282·7	R	BiO	
8230	R	FeO	
8226	M	P_2	
8217·1	R	IrC	
8192	R	ZrO	
8182	R	AgBi	
8164	R	BeS	
*8153·0	R	CaO	
8137·0	R, D	BaF	
8112	R	FeO	
8108·2	R	C_2	Phillips
*8097	R	H_2O	

λ	*App.*	*Mol.*	*System*	λ	*App.*	*Mol.*	*System*
8066·0	R	ScCl		7550·3	R, D	ArH	
8057·6	V	N_2	Herman I-R	7506·8	V	SiH	
8053·6	R, T	N_2^+	Meinel Aur.	*7503·9	V, T	N_2	1st Pos.
8020·9	V, DCD	NO	Ogawa	7468	M	H_2O^+	
7991·4	V	PO		7463	R	HCl	
7973·8	R, DCD	BS		7430	V	S_2	
7953·3	R, wv	BeO		7420·2	V, DCD	NO	Ogawa
7936·7	R	ScCl		7393·2	R	VO	
7919	M	NH_3		*7386·6	V, T	N_2	1st Pos.
7918·5	R	OH	Meinel	7379·8	R, D	LaO	
7915·2	R	SO		7348·0	V	SrH	
*7907·7	R	C_2	Phillips	7346·7	V	SrH	
7901	M	C_2H_2		7334·7	V	O_2^+	1st Neg.
7900	R	NiO		7330	R	NiO	
7899·3	R	PtC		*7318·5	R	CaO	
7896·0	R, wv	VO		7311·7	R	BS	
7877·2	R, D	LaO		7303·1	V	C_2O	
7874	M	C_2H_2		7299·5	R	PbF	
*7872·7	R, T, wv	CN	Red	7297·2	R	CeO	
7850·9	R, F	VO		7284·2	R	OH	Meinel
*7850·2	R, T	CN	Red	7282·1	V	C_2O	
7845	R	BiO		7277·3	R	BiO	
7831·8	R	CeO		7260·0	R	LaS	
7825·7	R, T	N_2^+	Meinel Aur.	7245·9	V, D	AlF	
7820·1	R	CO_2	Venus	7235·8	R	CeO	
7780	R	N_2	I-R Aft.	7210·4	R, F	CO	Asundi
7776·3	V	SbF		7200	R	TmO	
7763·1	V	PH_2		7173·1	V	PH_2	
7755·8	R	OH	Meinel	*7164·5	R	H_2O	
*7753·2	V, T	N_2	1st Pos.	7125·6	R	TiO	γ
*7714·6	R	C_2	Phillips	7116·0	R, D	BaF	
7674·4	R, wv	ArH		7083·2	V	C_2	High P.
7672·1	R	TiO	γ	7081·8	R	PbS	
7662·8	R	PrO		7069·6	V	S_2	
7633·7	R	ScCl		7051·0	R	LaS	
*7626·2	V, T	N_2	1st Pos.	7036·8	R, T	N_2^+	Meinel Aur.
*7593·7	R	O_2	Atmosph.	7029·6	R	PbCl	
7591	R	N_2	I-R Aft.	7028·4	V	NCl	
7588·6	R	PbF		7018·1	V	SrH	
7570·1	R	PtC		7011	R	NdO	

λ	App.	Mol.	System
6987	M	H_2O^+	
6983·8	V	S_2	
6984·7	V	SrH	
6960·4	R	IrC	
6942·6	V, wr	CaH	
6936·5	R	OsO	
6936·5	R	BiO	
6931·6	V	SrI	
6926·1	R	NiCl	
6921·9	R	PbCl	
6918·3	R	BaS	
6898·4	V, DCD	NO	Ogawa
6896	R, T	N_2	I-R Aft.
6894·3	R, wv	SnH	
6891·6	R	MnF	
6879	R	OH	Meinel
6876·4	O	PbS	
6872·9	R	Rb_2	
6870·4	R	PbH	
*6867·2	R	O_2	Atmosph.
6866·4	R	HfI	
*6856·3	V	O_2^+	1st Neg.
6850·2	V, F, wr	BaH	
6820	M	SrOH	
6818·7	R	PbCl	
6804·0	R, F	CO	Asundi
6800·2	V	SrBr	
6797·8	R	Rb_2	
6782·8	R	CaS	
6778·8	V	SrI	
6777·3	R	BaS	
6775·7	R	Rb_2	
6763·3	R	RaCl	
6747·2	V	SrI	
6744·9	V	SrCl	
6718·8	R	VCl	
6708·8	R	BiO	
*6704·8	V, T	N_2	1st Pos.
6689·5	V, D	BaH	
6686	M	H_2O^+	
6676·3	R	PbTe	
6675	M	SrOH	
6666·7	V	SrBr	
6659·6	V	BiS	
6655·6	V, D	SrF	
6652	M	NH_2	Ammonia α
6646·7	V, D	NCl	
*6631·3	R, T, wv	CN	Red
6625	M	NO_3	
*6623·6	V, T	N_2	1st Pos.
6613·7	V, wr	SrCl	
6612·1	R	IrCl	
6607·6	R	RaCl	
6594	M	H_2O^+	
6590·2	V	YbH	
6590	M	SrOH	
6585·2		NdO	
6578·3	R	CaS	
6576·3	R	YCl	
6569	R, F	TiO	
6561·5	R	Na_2	
6549·3	R	IF	
*6544·8	V, T	N_2	1st Pos.
6542	M	H_2O^+	
6533·5		SmO	
6522·5	R	AsS	
6521·7	R	PbTe	
6517·2	R	F_2	
6513·5	R, F	CO	Asundi
6513·2	R	Na_2	
6513·0	V	SrBr	
6510·9		SmO	
6509·4	R	MoO	
6498·1	R	RaCl	
6494·8	R	NbO	
6493·1	R	BaO	
6485·8	R	Pb_2	
6481·2	R	IF	
*6478·5	R, T, wv	CN	Red
6474·1	V	FeCl	

λ	App.	Mol.	System
6473·7	R	ZrO	γ
*6468·5	V, T	N_2	1st Pos.
6460	M	SrOH	
6457·5	R	H_2O	
6445·4	R	MoO	
6425·1	R	NiH	
*6418·7	V	O_2^+	1st Neg.
6418·4	R	Na_2	
6417·5	R	Pb_2	
6412·9	V	CaI	
6406·3	R	RuO	
6406·1	R	CaS	
6405	R	BrF	
*6401·0	R, T	CO	Triplet
6398·7	R	He_2	
*6394·7	V, T	N_2	1st Pos.
6394·3	R	CrO	
6389·3	V	CaH	
6388·8	V	CaI	
6383·8	R	AgSb	
6377·8	V, DCD	NO	Ogawa
6370·4	R	Pb_2	
6368	R	O_2	Liquid
6362·4	V	SrCl	
6349·5		SmO	
6342·2	R	NiO	
*6322·9	V, T	N_2	1st Pos.
6315·4	V	CaI	
6302	M	NH_2	Ammonia α
6301·5	R	AsS	
6293	R	BrF	
6283·6	R	Tl_2	
6277·7	V, wr	CaBr ?	
6277·2	V, D	MnBr ?	
*6276·6	R	O_2	Atmosph.
6272·0	V	AlAu	
6265·9	V	NBr	
6263·3	R	CuTe	
6261·7	V, D	NCl	
6258·5	V	–	Ca oxide
6257·8	V, D	MnBr ?	
6252·9	V, wr	CaBr ?	
*6252·8	V, T	N_2	1st Pos.
6249·3	R	IF	
6246·0	R	NiH	
6244·7	R	MoN	
6233	M	NO_3	
6230	M	CaOH	
6229·4	R, T	ZrO	γ
6228·5	R	MoN	
*6224·9	V, DCD	CaCl	
6219·8	R	FeO	
6216·0	R	NaRb	
*6211·6	V, wr	CaCl	
6211·5	R	ScF	
6210·6	R	PtO	
6210	M	H_2O^+	
6205·5	R	HfBr	
6199·5	R	TiN	
6199	M	H_2O^+	
6196·0	V	$ZnTl_2$	
*6189·4	R, D	CO^+	Comet-t.
*6184·9	V, wr	CaCl	
6180·5	R	FeO	
6174·4	R, D	NbO^+	
6165·7	R	H_2O	
6161·6	R	CuO	
6159·1	R, CT	TiO	α
6158	M	H_2O^+	
6149·9	R	SnBr	
6148·5	O	InH	
6144·7	V	AlAu	
6138·6	R, D	TiN	
6138·0	R, D	CHO	
6122·9	R	AgSb	
6117·5	V	BiH	
6116·3	R	CuSe	
6110·7	R	MoN	
6109·9	M	FeO	
6105·9	R	PbI	

λ	App.	Mol.	System
6103·7	M	CrCl	
6102·8	R	F_2	
6098	R	AgBi	
6097·3	M	FeO	
6097	V	–	Ca oxide
6096·8	R, D	YO	
6095·0	R	SnH	
6092·0	R	AsS	
*6086·9	V, DCD	CaF	
6086·4	R, D	VO	
6084·7	V, CD	SrOH	
*6079·9	V	CO	Angstrom
6076·6	R	TbO	
6076·6	V	SrOH	
6073	V	La_2	
*6064·4	V, wr	CaF	
6063·9	V	FeCl	
6060·3	V	MgO	
6059·3	R	CuO	
6051·6	R	CrO	
6050	M	SrOH	
6047	V	La_2	
6045·0	R	CuO	
6043·2		NbO^+	
6039·6	R	BaO	
6036·1	R, D, wv	ScO	
6031·1	R	IF	
6028·6	R, D	NbO^+	
*6026·4	V	O_2^+	1st Neg.
6021·9	R	SnH	
6017·5	V	AlAu	
*6006	V	–	Ca oxide
6004·6	R	Br_2^+	
*6003	R	–	Ca oxide
6001	O	NO	
5997·6	V, T	YbH	
5991	M	PHO	
5990·7	V	NBr	
5989·5	V	FeCl	
*5983	R	–	Ca oxide
*5982	R, T	CO	Triplet
5979·9	R	TbO	
5977·7	V	FeBr	
5969	R	–	Sr oxide
5962·4	V	NBr	
*5959·0	V, T	N_2	1st Pos.
5957·1	V	FeBr	
5950	M	–	Sr oxide
5949·4	R	SbO	
5939·1	R, D	YO	
5938	R	–	Sr oxide
*5934·0	R	CaCl	
5933·8	V	NBr	
5923·9	R	BrF	
5920·8	R	TbO	
5916·0	R, D	NbO^+	
5914	M	H_2O^+	
5913·8	L	InH	
5910·7	R	PbO	
*5906·0	V, T	N_2	1st Pos.
5905·0	V	NBr	
5902·3	R	PtO	
5899·3	V	C_2	High P.
5893	M	NO_3	
5880·6	R	Br_2^+	
5869·2	R	BiO	
5868·1	R	FeO	
5864·5	R	BaO	
*5858·2	R, T, wv	CN	Red
*5853·1	R	MnO	
5852·6	R	F_2	
5847	R, F	TiO	γ′
5845·7	R	PbI	
5835	R	ZrN	
5834·8	R	DyO	
*5830	R	CaF	
5829·7	R	FeBr	
5827·5	R	SnF	
5827	M	H_2O^+	
5815·1	V, wr	N_2	Gaydon G.

λ	App.	Mol.	System	λ	App.	Mol.	System
5808	V	P_2		*5635·5	V	C_2	Swan
*5804·3	V, T	N_2	1st Pos.	*5631·9	V	O_2^+	1st Neg.
5804·1	R	BrF		5629·3	R, D	TiO	β
5802·2	R	BiI		*5610·2	V	CO	Angstrom
5800·9	R	Al_2		5609·5	V	BaI	
5799·8	R	RuO		5599·9	R, CD	LaO	
5799	M	H_2O^+		5597·6	R, D	TiO	β
5789·8	R	FeO		5597	M	PHO	
5789·6	R	SnO		5596	M	ErO	
5772·0	R, CD	SrF		5595·0	V, F	N_2	Gaydon G.
5763·5	O	GaH		5593·5	R, DCD	BS	
5752·4	V	FeCl		5589	R	TaO^+	
5736·7	R, D	VO		5586·2	R	PF	
5731·7	R	PbTe		5584·7	R	PO	
5731·4	R	F_2		5582·2	R	MnO	
5728·2	R	NaK		5574·8	V, wr	N_2	Gaydon G.
5718·1	R	ZrO	β	5574·6	R	CuS	
5713	M	NH_2	Ammonia α	5574·1	R	CuSe	
5712·1	R	CuS		5572·3	R	SnBr	
5710·1	R	SnTe		5570	M	ScH	
5706·2	O	TlH		5561·1	R	SnCl	
5699·9	R	Br_2^+		5561·0	O	PbH	
5697·7	V, D	GaH		*5547·4	M	CaOH	
5696·2	O	RbH		*5542·6	M	CaOH	
5696	V	HoO		5540·5	R	AsSe	
5694·3	V	CuF		*5538·6	M	CaOH	
5691·1	R	PrO		5529·5	R	NiO	
5688·6	O	InH		5525·8	R	RuO	
5687·8	R	ScCl		5506·8	R, D	SnF	
5678·9	R	ZnO		*5498	R	–	Ca oxide
5677·5	V, F	MnH		5497·3	R	SnBr	
5668·3	R	SnCl		5492·7	R	BaO	
5667·8	R	CoCl		5489	M	H_2O^+	
5663·0	R	PtO		5473	R	–	Ca oxide
5661·5	R, D	TiO	β	5470·3	R	NbO	
5660	M	HoO		5469·3	R, D	VO	
5648	R	ZrN		*5461·4	R, wv	CO^+	Comet-t.
5644·1	R	BaO		5459·4	R	PbO	
5640·2	V, T	YbH		*5458·7	M	CuOH	
5635·9	R, D	SnF		5457·1	R	SnCl	

λ	App.	Mol.	System
5450	M	BO_2	
5448·3	R, CT	TiO	α
5442·7	R	SiBr	
5440·9	R	MnS	
*5418·6	M	CuOH	
5415·9	V	C_2^-	
5399·5	R	PtC	
5382	V	TiH	
5381·7	V	BaI	
5376·0	R	XeO	
*5372·8	V, T	N_2	1st Pos.
5372·6	R	PbSe	
5370	V	TiH	
5368	R	NaRb	
5364	R	O_2	Liquid
5361	V	TiH	
5360·1	R	BaBr	
5359·6	R	MnO	
*5356·5	M	CuOH	
5352	R	TmO	
5347	R	TmO	
5346·6	R	AuCl	
5341·2	R	AsSe	
5334·3	V, DCD	NO	Ogawa
5333·8	R	SbCl	
5331·0	R	SnSe	
5325·1	R	PbSe	
5307·3	R	IO	
5300·8	R	MnS	
*5295·7	V	O_2^+	1st Neg.
5293·4	R	Bi_2	
*5291·0	R	CaF	
5287·8	V, L	NF	
5283·2	R, DCD	BS	
5278·7	R	PbSe	
5277·7	R	SbO	
5273·4	R	DyO	
5268·9	O	RbH	
5267·8	R, DCD	AlCl	
5263·4	R	DyO	
*5262·3	R	CuCl	
5258·2	R	Bi_2	
5248·7	M	PHO	
5240·8	R	Au_2	
5240·5	R	BaCl	
5240·0	R	AuCl	
5236·0	R	SbCl	
5226·4	V	HgIn	
5224·1	R	Bi_2	
5213·9	R	PS	
5211·0	V, D	MgH	
5208·2	R	BaBr	
5205·5	R	AuCl	
5200·9	R	NbO	
5199·8	R	MnS	
*5198·2	V	CO	Angstrom
5193·8	R	IrC	
5189·5	R	Au_2	
5185·0	R	ZrO	
5180·1	R	SnSe	
5180	M	BO_2	
5174·5	R	NiO	
5172·7	V	HgIn	
*5172·6	R, D	SiN	
5171·4	R	LuO	
5166·9	R, CT	TiO	α
*5165·2	V	C_2	Swan
5162·2	R	SiCl	
5158·6	R	PbSe	
5148·0	R	SnO	
*5145·4	R, CD	CaF	
5141·1	R	CuI	
5139·2	V	BaCl	
5134·0	R	SbS	
5132·6	R, D	SnF	
5123·5	R	OH	Schuler-W
5120	M	BaOH	
5102·6	R	NSe	
5088·6	R	PtH	
*5079·4	R	AlO	