

REPORT ON NOTATION FOR ATOMIC SPECTRA*

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AT AN informal meeting of spectroscopists at Washington in April, 1928, the writers of this report were requested to draw up a scheme for the clarification of spectroscopic notation. After much discussion and correspondence with spectroscopists both in this country and abroad we are able to present the following recommendations.

The analysis of a spectrum can be of three different types. (1) A multiplet, or in many cases a level, analysis. This includes the determination of the types of terms (S , P , D , etc.), the multiplicities, and the inner quantum numbers of the individual levels when possible. (2) A configuration analysis. The description of the electron configuration with which the spectroscopic terms are to be correlated as given by Hund in his book. (3) A series analysis. The identification of series of terms and finding of their limits. A complete notation must be capable of adequately expressing the results of all three types of analysis whether complete or only partial.

MULTIPLY ANALYSIS

The proposed system of notation for a multiplet analysis is nearly the same as that which is now in general use. The type of term is denoted by the letters S , P , D , etc., to correspond to the quantum number L of Hund's theory.

Letter: S P D F G H I K L M N O Q R T U V W X Y Z
 L : 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

In the case of the rare earths it appears that there may occur terms of type Z . The multiplicity is denoted by a superscript at the left, 1 , 2 , etc. for singlet, doublet, etc., terms. The inner quantum number is used as a subscript at the right, $_0$, $_1$, $_2$, etc., for odd multiplicities, and $_{\frac{1}{2}}$, $_{\frac{3}{2}}$, etc. or $_{\frac{1}{2}}$, $_{1\frac{1}{2}}$, $_{2\frac{1}{2}}$, etc., for even multiplicities. The latter form is recommended because of its typographical advantages.

In all spectra the terms may be divided into two groups, even and odd, such that the terms of one group do not combine with one another (except for "forbidden" lines) but only with those of the other group. At present these groups are distinguished by the use of primes or bars (e.g., P' , \bar{P}) as follows.

Even terms: S P' D F' etc.
 Odd terms: S' P D' F etc.

It is now proposed to leave all even terms unmarked and to denote all odd terms by the superscript $^\circ$ (the symbol for degrees) at the right. The above terms would be written

Even terms: S P D F G
 Odd terms: S° P° D° F° G°

There are two reasons for this suggested change.

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(1) The distinction between odd and even terms has a physical basis. (The rules for determining whether a term is odd or even will be discussed below.)

(2) An unclassified level (type of term unknown) is shown to be odd or even by its combinations and can be so designated. This is not possible with the old notation.

It is suggested that, following a fairly general custom, unclassified levels be denoted by arabic numbers to which the indices for multiplicity, inner quantum number, etc., can be added when known (e.g. $^423_{1\frac{1}{2}}$). It is recommended that when such a number has once been assigned to a given level in a particular spectrum, it should not be changed until the level is classified. The number released by such a classification of a level should never be used for any other level in that spectrum.

The final result of a multiplet analysis should be expressed in two tables. First, a table giving all the energy levels, classified and unclassified, with the notation for each. In order to facilitate work by other investigators it is recommended that the odd terms be printed in heavy-faced type or in italics in this table. At least five different methods of arranging a table of terms may be found in the literature. We recommend that in this main table the individual levels be tabulated in order beginning with the lowest, irrespective of the extent to which the components of multiple terms may be intermingled. The placing together of those levels which are regarded by the author as being components of a multiple term introduces an element of individual and, perhaps, fallible judgment. It is to be avoided both for that reason and also because it obscures the overlapping of terms which may be of great theoretical importance. The typical term tables given below illustrate these points, and indicate a simple way of giving the necessary information concerning components of terms and the intervals between them. The second table should be a list of all the classified lines in the order of frequency giving for each the wave-length, wave-number, intensity, temperature-class when known, and origin, i.e., the combination between levels of the first table (the level of lower energy to be given first). For the sake of brevity it is recommended that one use as simple a notation as possible for differentiation of terms of the same type. This is usually done by prefixing lower case letters a^3D , b^3D , etc. It is not essential that the same system for assigning these letters should be used for all spectra but it is *very important* that a detailed explanation of the system should accompany every such table. It is recommended that the lowest terms and higher ones of the same type, multiplicity and parity, should be lettered a , b , c , etc., beginning with the lowest. The terms of the opposite parity of the same type and multiplicity should be labelled z , y , x , etc., beginning with the lowest. In this way all the resonance lines will be designated as $a()-z()$. By this scheme, lines of similar physical nature will have a similar designation. In accordance with this idea it is suggested that the letters a , b , c , d be reserved for low metastable terms and that the high terms should uniformly begin with e . It follows from the Hund theory that the number of low terms of the same character which

TABLE I. Term table for Ag II (Part of)

Level		Intervals (Higher J 's first)		
$5d^3S_1$	86405.0			
$5d^3G_5$	87496.6 *			
$5d^3G_4$	87509.2 *			
$5d^3P_2$	87596.3 . *			
$5d^3P_1$	87599.8 . *			
$5d^3D_3$	88041.1 . . *			
$5d^3F_3$	88320.6 . . . *			
$5d^3D_2$	88353.1 . . . *	3P	3.5	6304.7?
$5d^1S_0$	88356.9?	3D	312.0	3983.5
$5d^3F_4$	88437.9 . . . *	3F	-117.3	4664.4
$5d^1P_1$	91592.1	3G	12.6	4573.2
$5d^3G_3$	92082.4 *			
$5d^3D_1$	92336.6 . * .			
$5d^1G_4$	92346.6 . .			
$5d^1D_2$	92620.0 . .			
$5d^3F_2$	92985.0 . *			
$5d^1F_3$	93027.9 .			
$5d^3P_0$	93904.5? *			

TABLE II. Quartet term table for Cl III.

A	B	C	Level	Explanation of symbols		
				A	C	Configuration
aS	$a^4S_{1\frac{1}{2}}^\circ$	$3p^4S_{1\frac{1}{2}}^\circ$	321936.			
bP_1	$z^4P_{\frac{1}{2}}^\circ$	$z^4P_{\frac{1}{2}}^\circ$	222461. *			
bP_2	$z^4P_{1\frac{1}{2}}^\circ$	$z^4P_{1\frac{1}{2}}^\circ$	222806. *			
bP_3	$z^4P_{2\frac{1}{2}}^\circ$	$z^4P_{2\frac{1}{2}}^\circ$	223416. *			
$4kP_1$	$y^4P_{\frac{1}{2}}^\circ$	$4s^4P_{\frac{1}{2}}^\circ$	148200. *			
$4kP_2$	$y^4P_{1\frac{1}{2}}^\circ$	$4s^4P_{1\frac{1}{2}}^\circ$	147842.2 *			
$4kP_3$	$y^4P_{2\frac{1}{2}}^\circ$	$4s^4P_{2\frac{1}{2}}^\circ$	147322.1 *			
$4mD_1$	$e^4D_{\frac{1}{2}}^\circ$	$4p^4D_{\frac{1}{2}}^\circ$	120862.6 *			
$4mD_2$	$e^4D_{1\frac{1}{2}}^\circ$	$4p^4D_{1\frac{1}{2}}^\circ$	120604.0 *			
$4mD_3$	$e^4D_{2\frac{1}{2}}^\circ$	$4p^4D_{2\frac{1}{2}}^\circ$	120170.9 *	a	$3p$	$3s^23p^3$
$4mD_4$	$e^4D_{3\frac{1}{2}}^\circ$	$4p^4D_{3\frac{1}{2}}^\circ$	119568.4 *	b	z	$3s3p^4$
$4mP_1$	$e^4P_{\frac{1}{2}}^\circ$	$4p^4P_{\frac{1}{2}}^\circ$	117914.4 *	$4k$	$4s$	$3s^23p^24s$
$4mP_2$	$e^4P_{1\frac{1}{2}}^\circ$	$4p^4P_{1\frac{1}{2}}^\circ$	117812.0 *	m	$4p$	$3s^23p^24p$
$4mP_3$	$e^4P_{2\frac{1}{2}}^\circ$	$4p^4P_{2\frac{1}{2}}^\circ$	117394.8 *	n	$3d$	$3s^23p^23d$
$4mS$	$e^4S_{1\frac{1}{2}}^\circ$	$4p^4S_{1\frac{1}{2}}^\circ$	115997.3	$5k$	$5s$	$3s^23p^25s$
$4nD_2$	$z^4D_{1\frac{1}{2}}^\circ$	$3d^4D_{1\frac{1}{2}}^\circ$	80363.6 *			
$4nD_3$	$z^4D_{2\frac{1}{2}}^\circ$	$3d^4D_{2\frac{1}{2}}^\circ$	80250.9 *			
$4nD_4$	$z^4D_{3\frac{1}{2}}^\circ$	$3d^4D_{3\frac{1}{2}}^\circ$	79889.8 *			
$5kP_1$	$x^4P_{\frac{1}{2}}^\circ$	$5s^4P_{\frac{1}{2}}^\circ$	76984.5 *			
$5kP_2$	$x^4P_{1\frac{1}{2}}^\circ$	$5s^4P_{1\frac{1}{2}}^\circ$	76543.6 *			
$5kP_3$	$x^4P_{2\frac{1}{2}}^\circ$	$5s^4P_{2\frac{1}{2}}^\circ$	75798.8 *			

Column A. Bowen's notation. (Phys. Rev. **31**, 34, 1928).

Column B. Notation which would be used if the configurations were unknown or if the table were for a complicated spectrum.

Column C. A simple abbreviated electron configuration notation which would be logical in this case.

Both A and C require an explanatory table in every paper in which they are used.

are observable is never likely to exceed four, though five is theoretically possible in a few cases. The use of Greek letters or other notations may be found convenient by authors under special circumstances. But we would emphasize again the desirability that a clear explanation of such an individual notation should be published in *every* paper in which it appears.

Tables I and II are given as illustrations.

CONFIGURATION ANALYSIS

Following Hund, the individual electrons in an atom may be defined by two quantum numbers, "azimuthal" and "total." The former is expressed by use of the letters *s*, *p*, *d*, etc., the latter numerically in specific cases or by *n* in general. The following table gives the values of these quantities.

TABLE III. *Designation of quantum numbers.*

Literal designation	Azimuthal quantum number		
	<i>l</i>	<i>k</i> (Bohr)	
<i>s</i>	0	1	The total quantum number is equal to or greater than <i>l</i> +1, i.e., 1, 2, 3, . . . for <i>s</i> electrons, 2, 3, 4, . . . for <i>p</i> electrons, etc.
<i>p</i>	1	2	
<i>d</i>	2	3	
<i>f</i>	3	4	
<i>g</i>	4	5	
<i>h</i>	5	6	
etc.			

An electron is characterized, for instance, as a *6p* electron, 6 being the total quantum number, the letter *p* implying an *l* value of 1. It will be noticed that *4p*, *5s*, *3d*, etc., electrons are exactly equivalent to Bohr's *4₂*, *5₁*, *3₃*, etc. electrons. The spin of the electron need not be specified in describing configurations. The number of electrons of a given type in an atom may be expressed by an exponent (e.g., *3d⁵*). For a complete description of the relation between electronic configuration and spectroscopic terms reference should be made to Hund's book. In this connection, we recommend the use of the lower case letters *n*, *l*, *s*, *j*, *m* for the quantum numbers of an electron, and the capital letters *L*, *S*, *J*, *M* to designate the quantum numbers of a term (or level) of an atom, either ionized or neutral. The symbol "*N*" is not included because the total quantum numbers of electrons do not combine to give a resultant.

A complete specification of atomic structure in terms of electronic configuration would include all the inner electrons, e.g., for Fe in its normal state *1s²2s²2p⁶3s²3p⁶3d⁶4s²*. For ordinary spectroscopic purposes only those electrons "outside" an inert gas shell need be considered. A complete *np⁶* group, and all the groups which are normally completed earlier in the periodic table, can be neglected. Thus the notation for the normal state of Fe becomes *3d⁶4s²*. The *nd¹⁰* groups can be ignored from Ga, In, and Tl onward, and it is

probable that the rare earth group $4f^{14}$ can be ignored for atoms beyond Hf or Ta.

An example of the notation for a level and the configuration from which it arises is $3d^6 4s^2 {}^5D_4$, which represents the normal state of the iron atom. $2s^2 2p^3 {}^4S_{\frac{3}{2}}$ represents the low level of O II. For brevity, the total quantum numbers may be omitted when their values are the lowest which the particular sort of electron can have if not belonging to already completed shells. For example, $4s$, $4p$, $3d$, $4f$ in spectra from K I to Zn I and Ca II to Ga II, etc., are the s , p , d , and f electrons of lowest quantum numbers not belonging to completed groups. The $3p^6$ group is completed and the $3s^2$ and all the groups of smaller n have been previously completed, leaving $4s$, $4p$, $3d$, $4f$ still to be added. These last can therefore be represented by s , p , d and f respectively.

The normal state of Fe I would thus be designated as $d^6 s^2 {}^5D_4$, that of O II as $s^2 p^3 {}^4S_{\frac{3}{2}}$. For Ge I, in which the electron groups $3d^{10}$ and $4s^2$ may be regarded as completed the electrons to be represented by the letters alone would be the $5s$, $4p$, $4d$, and $4f$ electrons: and so on.

Odd terms arise from the configurations for which the sum of the l values for all electrons is odd, even terms from configurations for which the l sum is even. Since the l sum for completed groups is always even, only outer uncompleted groups need be considered. Even (odd) terms are those in which the number of p and f electrons together is even (odd). In the parts of the periodic table where s and d groups are being completed the lowest terms of all the atoms are even. Where p groups are being completed (and also in the rare earth f -group) the lowest terms are alternately odd and even. Except in the rare earth group the only spectra for which the normal state corresponds to an odd term are B I, N I, F I and C II, O II, Ne II etc. and the homologous spectra in later periods.

Permitted transitions are those in which the l of one electron changes by one unit, (and the l of another electron by 0 or 2 units, if two electrons change) so that all such transitions are between even and odd terms.

SERIES ANALYSIS

Series of terms arise from configurations in which one electron, keeping the same value of l , has successively higher values of n , the total quantum number. A configuration such as $3d 4s 4p$ theoretically belongs therefore to three different series in which either the d , the s , or the p electron takes higher total quantum numbers. In practice this complication is rare as there is almost always one electron which is more easily detached than the others, and is therefore the one to take the higher quantum numbers and give the series. An electron whose total quantum number is higher than those of the electrons discussed in the last section may always be regarded as the most easily detached, as may also one belonging to a group which is not represented in the configurations giving the low terms of the spectrum.

The limiting configuration (i.e., the one obtained by the removal of the electron which takes successively higher values of n to give the series)

usually gives multiple terms. Each separate level of these terms is the limit of certain sets of the individual levels of the multiple terms converging to the limit. It is suggested that the following notation be used to indicate such series and their limits. The configuration of the limit is to be represented as above, followed in parentheses by the notation for the particular type of term which is the limit for the series under consideration, then by the "running" electron, then by the notation for the term (or particular level) given by the whole configuration. For instance, $s^2p^5(^2P^\circ)ns^3P^\circ$ represents the series of $^3P^\circ$ terms of Ne which converge to the $^2P^\circ$ limit, $s^2p^5(^2P_{1\frac{1}{2}})ns^3P_2^\circ$ represents the series of $^3P_2^\circ$ levels of those $^3P^\circ$ terms which converge to the component $^2P_{1\frac{1}{2}}^\circ$ of Ne II as limit. In this particularly simple case the use of the notation for the limit would be of little value except for extreme explicitness. In more complicated cases, however, some such notation is necessary to avoid ambiguity. For instance, the s^2p^3 configuration of O II gives $^4S^\circ$, $^2D^\circ$ and $^2P^\circ$ terms. If we add to this one np electron to get terms of O I the $^4S^\circ$ term gives 5P and 3P , the $^2D^\circ$ gives 3P , 3D , 3F , 1P , 1D , 1F and the $^2P^\circ$ gives 3S , 3P , 3D , 1S , 1P , 1D terms. Thus, theoretically, the s^2p^3np configuration gives three 3P terms, two 3D terms, two 1P terms and two 1D terms. For distinguishing between them it is most convenient to use the notation suggested above. The three 3P terms would be written $s^2p^3(^4S^\circ)np\ ^3P$, $s^2p^3(^2D^\circ)np\ ^3P$, and $s^2p^3(^2P^\circ)np\ ^3P$.

The notation described is applicable to all cases where the running electron is unlike any other in the atom. But if no such singular electron exists, the Pauli exclusion principle must be applied to the electron groups and the number of terms is reduced. A discussion of the question of whether the terms due to such a structure can be considered as series members (i.e. whether $d^{10}\ ^1S_0$ is the first series member of the $d^9md\ ^1S_0$ sequence) is beyond the purpose of this report. As far as notation is concerned two types of configuration must be considered. The first type is one in which the atom contains, outside the rare gas shell, a single group of two or more p or d or f electrons, with or without an s^2 group in addition. The terms arising from such configurations need no limit designation since the electron configuration defines them unambiguously, e.g., $d^3s^2\ ^2D$, $d^2\ ^2F$, $p^2s^2\ ^3P$, $p^5\ ^2P^\circ$ etc. The second type of configuration mentioned above is one which contains more than one group of two or more p or d or f electrons, e.g., $p^2d^2s^2$, p^3d^2 , $d^4f^2s^2$. The method of dealing with such cases may be best explained by an example taken from Ti I. The configuration is $3d^24p^2$ from which there arise a great number of terms including several repetitions of the same multiplicity and name (i.e. five 3D terms, six 3P , etc.) which must be differentiated in the notation. The description of such sets of terms requires the specification of the term arising from the configuration d^2 and the term from the configuration p^2 which were involved in the production of the final result, i.e., we must state the terms which would result if either the p^2 or d^2 groups were removed from the atom. For instance the 3D terms would be

$$\begin{aligned}
& d^2(^3F)p^2(^3P)^3D \\
& d^2(^3P)p^2(^3P)^3D \\
& d^2(^1D)p^2(^3P)^3D \\
& d^2(^3F)p^2(^1D)^3D \\
& d^2(^3P)p^2(^1D)^3D
\end{aligned}$$

It is interesting and explanatory to notice that terms of this kind belong to sequences of the type $3d^24p^2$, $3d^25p^2$, etc., which would carry an atom through two ionizations at once. Such sequences are not known to exist; but, since these first terms do exist, it is necessary to have the notation to deal with them.

The notation here suggested appears to be as simple as any that will give an adequate statement of the known relations in a complex spectrum. Indeed, it is insufficient to take into account certain complexities which are anticipated in the rare earths and even in some of the simpler spectra. These complexities arise from the fact that two or more terms of identical multiplicity and name may result from the same restricted electron configuration (e.g. two 2D terms from d^3). But, as such terms have not as yet been found, they will not be considered here further.

When a satisfactory configuration analysis has been made, a full specification of the electrons and limits for each term should be given at least once. In many cases, perhaps in most, considerable abbreviation may be practical. In the simpler spectra, in fact, it is possible to abbreviate to such an extent that the electron structure may be used throughout a paper without becoming too cumbersome for reading or for printing. But it is emphasized that no paper should contain such abbreviations without a table giving the complete notation for which they are substituted.

It is obviously out of the question to use the complete notation in the analysis of a complex spectrum, especially in the extensive term and wavelength tables. In such cases it is recommended that, when the electron configurations are known, two additional tables be included in the paper; one giving against the arbitrary designations, such as a 3D , the specifications of the electron configurations as outlined above; and a second table giving the electron configurations in some structural order and the terms of the spectrum arising from them.

We should like to take this opportunity to thank our critics for their helpfulness in calling out attention to points which we had neglected and in suggesting different and more acceptable methods than those we originally proposed for dealing with some of these matters. The following physicists have contributed to the discussion of this subject either in conversation or by correspondence: E. Back, I. S. Bowen, Keivin Burns, M. A. Catalan, K. K. Darrow, T. L. de Bruin, A. Fowler, R. C. Gibbs, S. Goudsmit, W. Grotrian, F. Hund, C. C. Kiess, R. De L. Kronig, O. Laporte, A. B. McLay, J. E. Mack, W. F. Meggers, F. Paschen, W. Pauli, A. E. Ruark, A. Sommerfeld, J. T. Tate, H. C. Urey, H. E. White.

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