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Abstract

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ON THE SELECTION RULES FOR AN ELECTRONIC TRANSITION

FOR DIFFERENT TYPES OF COUPLING

Let us consider one-electron electric multipole transitions in which the configuration $l^q l'$ participates, in the shell l^q of which LS-coupling holds. Let this shell be characterized by quantum numbers $L_0 S_0$, which, with the one-electron angular momenta $l's'$, are coupled by different types of coupling into the resultant J. In addition to the long-known types of coupling LS and Jj, the Jl-coupling introduced in ([1]) and the LS_0-coupling introduced in ([2]) are also important from the physical point of view. We shall characterize these couplings by the intermediate quantum numbers T_1T_2, and denote the states of the configuration under consideration by $nl^q\alpha_0 L_0 S_0 n'l'T_1T_2JM$. T_1T_2 denote LS (for LS-coupling), LK (for LS_0), J_0K (for Jl), and J_0j' (for Jj).

The line strength for the transition $l^q l'$—$l^q l''$ has the expression

$$S(nl^q\alpha_0 L_0 S_0 n'l'T_1T_2J,\ nl^q\alpha_0 L_0' S_0' n''l''T_1'T_2'J') =$$

$$= \left|(\alpha_0 L_0 S_0 n'l'T_1T_2J \| T^{(k)} \| \alpha_0 L_0' S_0' n''l''T_1'T_2'J')\right|^2. \quad (1)$$

Here $T^{(k)}$ is a tensor representing the operator of an electric 2^k-pole, the case $k = 1$ (electric dipole transition) being of principal importance. The quantity on the right-hand side of (1) (the square of the submatrix of $T^{(k)}$) is the result of summation over the quantum numbers M and M', and also over the components of the tensor $T^{(k)}$. It is evident that (1) is a generalization of (1) from ([3]).

We express the right-hand side of (1) according to the formulas of Section 7 in ([4]), taking into account that T_1T_2 and $T_2'T_1'$ may represent the intermediate quantum numbers of all four types of coupling indicated above. In cases where T_1T_2 and $T_1'T_2'$ represent quantum numbers of different types of coupling, we use the transformation properties of functions of coupled angular momenta ([4]), and for carrying out the summation we use the formulas of Appendix 6 from ([4]). As a result of all this, the quantity S is expressed in terms of $6j$- and $9j$-coefficients. In addition to these j-coefficients, in 2 (out of 10) cases there appear $12j$-coefficients of the first and second kind. The conditions for nonvanishing of these j-coefficients give the selection rules for the transitions under consideration. For $6j$- and $9j$-coefficients the conditions for nonvanishing are the triangle properties, while in the case of $12j$-coefficients, in addition, quadrilateral conditions appear. These triangle and quadrilateral conditions require that 3 and 4 parameters, respectively, be able to be the sides of a triangle and a quadrilateral with integral perimeter. It is well known that the nonvanishing conditions for the submatrix of a spherical function also impose the parity condition for the perimeter in the case of the parameters l', l'', and k. The selection rules obtained are given in Table 1.

Table 1

Selection rules for the transition

$$l^q a_0 L_0 S_0 l' T_1 T_2 J \;-\; l^q a_0 L_0 S_0 l'' T_1' T_2' J'$$

1	1	3	4	5
$LS - LS$	$J_j - J_j$	$LS - J_j$	$LS_0 - LS_0$	$Jl - Jl$
$LS - L'S'$	$J_0 j' - J_0' j''$	$LS - J_0 j''$	$LK - L'K'$	$J_0 K - J_0' K'$
$\{LL'k\}\{SS'O\}$	$\{J_0 J_0' O\}\{j' j'' k\}$	$\{J_0 l' s' J\}\{S L_0 l'' J'\}$	$\{LL'k\}\{KK'k\}$	$\{KK'k\}\{J_0 J_0' O\}$
6	7	8	9	10
$LS - LS_0$	$LS - Jl$	$Jl - LS_0$	$LS_0 - Jl$	$Jl - J_j$
$LS - L'K$	$LS - J_0 K$	$J_0 K - LK'$	$LK - J_0 j''$	$J_0 K - J_0' j''$
$\{LL'k\}\{SL'J'\}$	$\{K\}\{KS_0k\}\{J_0 l' s' J\}$	$\{K\}\{S L_0 l''\}\{J_0' l'' K'\}$	$\{J_0 l' K\}\{L\}\{j''\}$	$\{J_0 J_0' O\}\{K\}\{j''\}$

Note. In all cases the conditions $\{JJ'k\}$ and $\{l'l''k\}$ hold; in the latter case the parity $l' + l'' + k$ is required.

In Table 1 the columns present the selection rules for transitions between the couplings indicated at the tops of the columns. The intermediate quantum numbers are indicated below. The parameters that must form a polygon are placed in braces. The generally known rules for J and l, which are repeated in all transitions, are therefore moved to the note.

Of chief interest are the selection rules for the intermediate quantum numbers, which are placed in the individual columns of Table 1. These rules fall into five groups. To the first group we assign those cases in which a change in the value of the quantum number is forbidden. This is the generally known case $\Delta S = 0$ in column 1. In addition, a prohibition of change occurs for J_0 in columns 2, 5, and 10. To the second group we assign those cases in which the selection rules are the same as for J; these are $\{TT'k\}$. Such cases include, for example, $\{LL'k\}$ in columns 1, 4, and 6. The third group comprises those cases in which the value of an intermediate quantum number is restricted by a triangle condition, the other two parameters of which are quantum numbers from another configuration, in which there is no such quantum number as serves as the first parameter of the triangle. Such rules are $\{SL'J'\}$ (column 6), $\{J_0l''K'\}$ (column 8), and $\{J_0l'K\}$ (column 9). The fourth group consists of those cases in which quadrilaterals serve as the selection rules (columns 3 and 7); their parameters are the quantum numbers of both (initial and final) configurations. Finally, the fifth group should include cases in which there is no restriction whatever on the values of the intermediate quantum number. Such quantum numbers are placed in separate braces (columns 3, 6, 8, 9, and 10).

The first two groups of selection rules present nothing new, since they correspond to those cases in which the same intermediate quantum numbers are present in both configurations. The remaining three groups of rules constitute new selection rules, for which the notion of selection is less characteristic, since the corresponding quantum numbers are present

only in one of the configurations. The transition can occur only in the case when the corresponding quantum number forms a triangle or quadrilateral with quantum numbers from the other configuration, except for the fifth group, where there are no such values of the quantum numbers.

The appearance of the indicated selection rules of a new type has important consequences. Thus, for example, let us consider columns 1 and 6. In the first case a change of the quantum number S is forbidden (the prohibition of an intercombination line). In the second case this S must form only a triangle with L' and I' from the second configuration, whereas the value K from the second configuration is not restricted at all. A consequence of this is the circumstance that a line which, in the case of the transition characteristic LS—LS, is an intercombination line, becomes allowed in passing to the transition characteristic LS—LS_0.

In view of the fact that the type of coupling depends on the degree of excitation of the electron, and the transition of this electron always changes the degree of excitation, the use of different types of coupling (in the initial and final configurations) is of great practical importance. Experiments may also serve to establish the dominant type of coupling, since the presence or absence of certain lines, which are not allowed or forbidden for all types of coupling, will help to establish the type of coupling. This applies especially to such cases in which the type of coupling of one of the configurations (initial or final) has already been established. For example, from experimental data it is clearly seen that the configuration $2p3dNII$ is well characterized by LS-coupling. A study of the presence or absence, as well as of the intensities, of individual lines in the transitions $2p3d$—$2pnl$ will help to establish the type of coupling with $2pnl$, or the degree of superposition of one upon another, if the states can be characterized only by intermediate coupling.

It should be noted that the selection rules may also be borrowed from Table 1 for the transition l^q—$l^{q-1}l'$, if LS-coupling is realized in the shells l^q and l^{q-1}. For this purpose it is necessary to generalize formula 8 from [3] in a manner analogous to that used in obtaining [1], and to refer to columns 1, 3, 6, and 7 of Table 1.

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Note: Figure translations are in progress. See original paper for figures.