Mel Gorman
University of San Francisco
San Francisco, California 94117

Rules for Writing Ground State Russell-Saunders Symbols

Since the advent of crystal and ligand field theories the use of Russell-Saunders symbols has become increasingly common in the inorganic literature. But it is highly probable that most students will have had little or no familiarity with term symbolism when they enter the first course in inorganic chemistry in their junior or senior year. Whereas this course seems to be an appropriate place for the subject, it is unfortunate that there are so few sources which summarize the simple rules for writing the ground state symbols of free atoms and ions. The rules and examples to be presented here are an extension of those given in the books by Drago (*1*) and Figgis (*2*). Both of these are written at an advanced level; Drago states specifically (p. x) that his text should be used only after an introductory inorganic course has been completed. So it is possible that many students and teachers will be unaware of these sources for Russell-Saunders information.

In what follows it is presumed that the student has been apprised of interelectronic repulsion and the vectorial nature of orbital and spin angular momenta. As a first consequence of such knowledge it is evident that the net angular momentum of electrons in filled levels and sublevels is zero, and hence attention need be directed only to partially completed levels. The tabulation below may then be used to write the ground state of a free atom or ion. Atomic spectroscopy formalism is kept to a minimum.

1. Write the electronic configuration of incomplete sublevels.
2. List horizontally the m_l values (m_l is the quantum number corresponding to the component of the orbital angular momentum along a reference direction for a single electron) for the relevant incompleted *s, p, d* and *f* levels, beginning at the left with the highest value, i.e., $s = 0$, $p = 1$, $d = 2$, $f = 3$.
3. Fill the orbitals represented in step 2 with the available electrons indicated in step 1. Single electrons are added to each orbital before any pairing is done, beginning at the left. When pairing is necessary, it also is started at the left. This step is an exemplification of Hund's rules for maximizing the total orbital angular momentum (step 4) and the spin multiplicity (step 5), thus minimizing repulsion, for the ion or atom as a whole.
4. The m_l's of unpaired electrons are added to get a resultant, M_L. This addition is performed algebraically, but if M_L is negative the minus sign is dropped. The numerical value of M_L is assigned a letter corresponding to the scheme 0, 1, 2, 3, 4, 5, 6, 7, . . . 20, equivalent to, respectively, *S, P, D, F, G, H, I, K, . . . Z* (note the absence of *J*) (*3*).
5. The spectroscopist's spin multiplicity is indicated by a number which is one more than the number of unpaired electrons. It appears as a pre-superscript in the examples.

Examples. Write the term symbols for the ground states of the following free atoms or ions.

Oxygen atom
(1) $2p^4$
(2) m_l = 1 0 −1
(3) ⇅ ↑ ↑
(4) $M_L = -1$, a *P* state
(5) Multiplicity = 2 + 1, a triplet, ^3P

Phosphorus atom
(1) $3p^3$
(2) m_l = 1 0 −1
(3) ↑ ↑ ↑
(4) $M_L = 0$, an *S* state
(5) Multiplicity = 3 + 1, a quartet, ^4S

Titanium (III)
(1) $3d^1$
(2) m_l = 2 1 0 −1 −2
(3) ↑
(4) $M_L = 2$, a *D* state
(5) Multiplicity = 1 + 1, a doublet, ^2D

Chromium atom
(1) $3d^5 4s^1$
(2) m_l = 2 1 0 −1 −2
(3) ↑ ↑ ↑ ↑ ↑
(2) m_l = 0
(3) ↑
(4) Total $M_L = 0$, an *S* state
(5) Multiplicity = 6 + 1, a septuplet, ^7S

Nickel (II)
(1) $3d^8$
(2) m_l = 2 1 0 −1 −2
(3) ⇅ ⇅ ⇅ ↑ ↑
(4) $M_L = -3$, an *F* state
(5) Multiplicity = 2 + 1, a triplet, ^3F

This scheme applies even to those cases where some type of spin orbit coupling must be considered (*4*), as in the following examples.

Gadolinium atom
(1) $4f^7 5d^1$
(2) m_l = 3 2 1 0 −1 −2 −3
(3) ↑ ↑ ↑ ↑ ↑ ↑ ↑
(2) m_l = 2 1 0 −1 −2
(3) ↑

(4) Total $M_L = 0$ (f sub-level) + 2 (d sub-level) = 2, a D state
(5) Multiplicity = 8 + 1, a nonet ^9D

Uranium atom
(1) $5f^3 6d^1$

$$\begin{array}{lccccccc} (2)\ m_l = & 3 & 2 & 1 & 0 & -1 & -2 & -3 \\ (3) & \uparrow & \uparrow & \uparrow & & & & \end{array}$$

$$\begin{array}{lcccccc} (2)\ m_l = & & 2 & 1 & 0 & -1 & -2 \\ (3) & & \uparrow & & & & \end{array}$$

(4) Total $M_L = 6$ (f sub-level) + 2 (d sub-level) = 8, an L state
(5) Multiplicity = 4 + 1 = 5, a quintuplet, ^5L

In general, ground states may be comprised of a group of substates with different values of the total orbital and spin angular momentum quantum number, $J = M_L \pm S$, where S is the sum of spin quantum numbers for the unpaired electrons. As with M_L calculated above, absolute values of S are employed. If a subshell is half-filled, $M_L = 0$, so there is only one possible value for J; e.g., 5/2 for a half-filled d subshell. If the subshell is more than half-filled, $J = M_L + S$; if less than half-filled, $J = M_L - S$. J is written as a subscript. Thus the complete symbols of the examples already given are: O atom, $^3P_2$; P atom, $^4S_{3/2}$; Ti (III), $^2D_{3/2}$; Cr atom, $^7S_3$; Ni (II), $^3F_4$; Gd atom, $^9D_2$; U atom, $^5L_6$. For the last two calculate J separately for f and d sublevels, then add.

It should be remembered that these rules apply only to the ground state. The calculation of the number of allowed higher states for a given configuration is rather laborious. The methods and results are given by various authors *(5)*. But the order and separation of the higher states with respect to each other and to the ground state cannot be determined in a simple manner. Also, it must be emphasized that these rules are not absolute and that there are exceptions *(4)*.

Literature Cited

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