

PERIODIC TABLE

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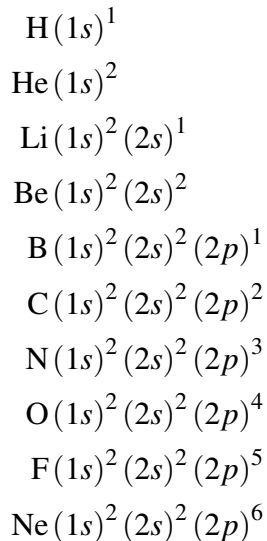
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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.12.

Because electrons are fermions, no two electrons within an atom can be in the same state. If we could model all atoms in the same way as we did for helium, we could write the wave function as a product of Z hydrogen-like wave functions, one for each of the electrons in an atom with atomic number Z . Since the spatial hydrogen wave function is determined by the three quantum numbers n , l and m and for each value of n , we can have $l = 0 \dots n - 1$ and for each value of l we can have $m = -l \dots +l$, for a given n there are $\sum_0^{n-1} (2l + 1) = n(n - 1) + n = n^2$ different wave functions. Each of these spatial functions can accommodate 2 electrons (because there are two spin states), so for an atom with atomic number Z , we can fill the states from $n = 1$ upwards in pairs until we use up all the electrons.

In the Bohr model of hydrogen, the energy of a state depends only on n , but in reality, there is some splitting of the various levels depending on l . Crudely speaking, a larger l (remember l is angular momentum) means the electron is further from the nucleus, so is shielded from the positive charge of the nucleus by the intervening electrons, meaning its interaction energy is less (less negative, that is; a lower l means a lower energy because the energy is more negative). Thus states with lower l will be favoured for a given value of n , meaning that lower l states are filled first.

These rules allow us to figure out the electron configuration of the first few elements, but for larger atoms the screening effect is strong enough that it disrupts the order in which states are filled. However, up to element 10 (neon) we're safe enough. The common way of denoting electron configurations is to use the number of n followed by an obscure letter indicating the value of l . The first few letters are: s for $l = 0$, p for $l = 1$, d for $l = 2$ and f for $l = 3$. Thus hydrogen's configuration is $(1s)^1$, indicating $n = 1$, $l = 0$ with the superscript 1 meaning that one electron is in this state. The first 10 elements in this notation are



The total angular momentum of an atom is the combination of the total orbital angular momentum and total spin of the electrons. The maximum orbital angular momentum can be found by just adding up l for each electron; the *actual* orbital angular momentum L can then be any integer from 0 up to this maximum. The total spin can be worked out by remembering that any two electrons in the same spatial state must have opposite spins, so such a pair of electrons has total spin 0. Unpaired electrons contribute a spin of $1/2$ to the maximum total spin S . The overall total is given the symbol J . The total angular momentum of an atom's electrons is written using the notation $^{2S+1}L_J$.

For the first four elements, things are quite easy since they involve only s shells, which have $l = 0$, thus L for these elements is always 0. For hydrogen, the single electron means $S = \frac{1}{2}$, so $J = L + S = \frac{1}{2}$ and hydrogen's state is written as $^2S_{1/2}$ where the capital S means $L = 0$.

In helium, the two paired electrons give $S = 0$ so $J = L + S = 0$ and the state is 1S_0 .

In lithium, the one unpaired electron in the $2s$ shell gives $S = \frac{1}{2}$ so $J = \frac{1}{2}$ and the state is $^2S_{1/2}$ (the same as hydrogen).

For beryllium, all electrons are paired so $S = 0$ and we're back to a state of 1S_0 (the same as helium).

Once we introduce p electrons, things get more complicated, since $L \neq 0$ (meaning we have more than one possibility) and if we have two or more such electrons, they may or may not be paired (meaning S can have more than one value in some cases).

For boron, the single p electron means $L = 1$ or $L = 0$. The first four electrons are paired, but the extra electron means $S = \frac{1}{2}$. Thus $J = \frac{1}{2}, \frac{3}{2}$ and the possible states are ${}^2P_{1/2}$ and ${}^2P_{3/2}$.

Carbon has a maximum L of 2, so there are three possible orbital states: 0, 1, 2. The spin can be 0 (opposite spins for the two p electrons) or 1 (same spins) so the possible combinations are:

S	L	States
0	0	1S_0
0	1	1P_1
0	2	1D_2
1	0	3S_1
1	1	${}^3P_0, {}^3P_1, {}^3P_2$
1	2	${}^3D_1, {}^3D_2, {}^3D_3$

Nitrogen has a maximum L of 3. The spin could be $3/2$ if all three electrons are parallel, or $1/2$ if two of them have opposite spins. Thus the possible combinations of $L = 0, 1, 2, 3$ and $S = \frac{1}{2}, \frac{3}{2}$ are:

S	L	States
$\frac{1}{2}$	0	${}^2S_{1/2}$
$\frac{1}{2}$	1	${}^2P_{1/2}, {}^2P_{3/2}$
$\frac{1}{2}$	2	${}^2D_{3/2}, {}^2D_{5/2}$
$\frac{1}{2}$	3	${}^2F_{5/2}, {}^2F_{7/2}$
$\frac{3}{2}$	0	${}^4S_{3/2}$
$\frac{3}{2}$	1	${}^4P_{1/2}, {}^4P_{3/2}, {}^4P_{5/2}$
$\frac{3}{2}$	2	${}^4D_{1/2}, {}^4D_{3/2}, {}^4D_{5/2}, {}^4D_{7/2}$
$\frac{3}{2}$	3	${}^4F_{3/2}, {}^4F_{5/2}, {}^4F_{7/2}, {}^4F_{9/2}$

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