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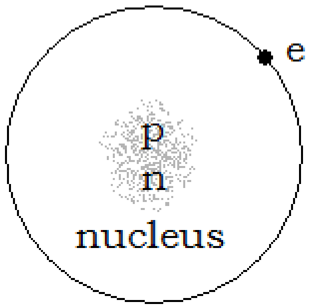
Electron Configuration

This tutorial is an investigation of the way in which electrons occupy the ground-state energy levels in the atoms of successive elements which are displayed in the periodic table.

The way in which the orbits are occupied in the atoms of successive elements is described by an empirical rule known as Madelung's rule.

The simplest model of the atom pictures electrons orbiting the nucleus.
This is known as Bohr's model.

Start with the hydrogen atom: $^{1}_{1}H$



[p = proton, n = neutron, e = electron]

The lowest energy state of the hydrogen atom, known as the ground-state, has an electron which is in the lowest orbit.
This orbit corresponds to an energy level which is labelled as n = 1.

The energy levels are, in fact, quantised so that electrons can jump between different energy levels when given specific amounts of energy.

The principal orbits, which represent energy levels, are labelled using the principal quantum number n (where n = 1, 2, 3, 4 ...).
These principal quantum numbers describe the electron "shells".

A more sophisticated model (Schrödinger's model) shows that the principal energy levels are split which means that electrons can occupy sub-levels.
These sub-levels represent different angular momentum states that an electron can have.

These angular momentum states are described using L (the azimuthal quantum number).

For each principal energy level n the allowed L values are: (n – 1), (n – 2) 0

The maximum value of the azimuthal quantum number L , for a given principal energy level n, is: $L_{max} = (n - 1)$

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Spectral Lines

The letters s, p, d, f are used to label the different L sub-levels.

L value	Spectral label
0	s
1	p
2	d
3	f

[These labels originate from the analysis of spectral lines.

s = sharp, p = principal, d = diffuse, f = fundamental (or fine) ... then alphabetically g, h, i ... etc.

The crucial link between electron orbits and spectral lines is that when an electron drops from an energy level to a lower one a photon is given off. The wavelength of the released photon is determined by the energy difference between the levels. Spectral lines which correspond to particular energy differences may be used to identify elements.]

The energy levels are further split, as described by the magnetic quantum number m, which means that further occupancy of each principal orbit is allowed.

For each value of L the quantum number m can take the values: L, (L – 1), (L – 2) ... 0 ... - (L – 2), - (L – 1), - L

L value	Allowed m values	Number of states
0	0	1
1	1, 0,-1	3
2	2, 1, 0, -1, -2	5
3	3, 2, 1, 0, -1, -2, -3	7
L	L, (L – 1) (L – 2), ...0, ... -(L – 2), -(L – 1), -L	2L + 1

Consequently for each L level there are (2L + 1) further sub-levels .

On top of all this the electron can have spin-up or spin-down so the total number of sub-levels for each L level is: 2 (2L + 1).

So this gives the maximum number of electrons in a sub-shell as: 2 (2L + 1).

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Atomic Orbitals

Now examine the maximum number of electrons in the energy levels.

Principal orbit	Allowed L values	Level label	Number of sub-levels 2 (2L + 1)	Maximum Number of Electrons in the n level
n = 1	L = 0	1s	2	2
n = 2	L = 1	2p	6	8
	L = 0	2s	2	
n = 3	L = 2	3d	10	18
	L = 1	3p	6	
	L = 0	3s	2	
n = 4	L = 3	4f	14	32
	L = 2	4d	10	
	L = 1	4p	6	
	L = 0	4s	2	

Note that an atom's n^{th} shell can accommodate $2\,n^2$ electrons.

Now consider the way in which electrons occupy the ground-state energy levels in the atoms of successive elements in the periodic table.

Madelung's rule (which is an empirical rule)describes the way in which electrons fill the atomic orbitals.

According to Madelung's rule:

1. Orbitals are filled in the order of increasing (n + L)
2. Where two orbitals have the same value of (n + L) they are filled in order of increasing n.

Orbital	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	6s	6p	6d	7s	7p
n + L	1	2	3	3	4	5	4	5	6	7	5	6	7	8	6	7	8	7	8

[Note: The levels 6f, 7d, 7f are not occupied by electrons in any of the elements known so far.]

Order of filling the orbitals according to Madelung's rule

Orbital	1s	2s	2p	3s	3p	4s	3d	4p	5s	4d	5p	6s	4f	5d	6s	7s	5f	6d	7p

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The maximum number of electrons in the orbitals.

Orbital	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	6s	6p	6d	7s	7p
Electron capacity	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	10	2	6
n-orbitals	2	8		18			32				32				18			8	

Note that the total number of electrons in the n-orbitals = 2 + 8 + 18 + 32 + 32 + 18 + 8 = 118 and the heaviest atom known so far has 118 electrons. In the future as more atoms are discovered other orbitals will come into play. For example, the levels 6f, 7d, 7f 8s etc.]

It turns out, that for atoms of some elements in the ground-state, some outer orbits contain electrons before inner orbits are filled.

Consequently the orbitals are labelled with the number of electrons which they contain.

Examples: $3d^2$ shows that there are 2 electrons in the 3d orbital and $4f^1$ shows that there is 1 electron in the 4f orbital.

A list of the electron configuration of the atoms of all the known 118 elements is given in the file: Electron Configuration.

Violations of Madelung's Rule

Recall: Order of filling the orbitals according to Madelung's rule

Orbital	1s	2s	2p	3s	3p	4s	3d	4p	5s	4d	5p	6s	4f	5d	6p	7s	5f	6d	7p
Electron capacity	2	2	6	2	6	2	10	6	2	10	6	2	14	10	6	2	14	10	6

The ground-state energy levels of the first 18 elements of the periodic table are filled in accordance with Madelung's rule.

So the electron configuration of argon $_{18}$Ar is: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ (This can be abbreviated as: [Ar])

The electron configuration of calcium $_{20}$Ca is: [Ar] $4s^2$ as described by Madelung's rule.

According to Madelung's rule the filling of the atomic orbitals of the next ten elements would involve adding 10 electrons, in turn, to the 3d orbital.

This works for the next 3 elements up to vanadium $_{23}$V which has the electron configuration: [Ar] $3d^3\ 4s^2$

However, Madelung's rule breaks down, for the first time, for element chromium $_{24}$Cr.

Violation 1: Madelung's rule would give the electron configuration as: [Ar] $3d^4\ 4s^2$ but the actual configuration is: [Ar] $3d^5\ 4s^1$

So not only is the fourth electron added to the 3d orbital, another electron is "pinched" from the 4s orbital to give 5 electrons in the 3d shell. An explanation for this is that half-filled shells are more stable. So the chromium atom arranges the electrons to make the 3d shell half-full.

For manganese $_{25}Mn$, the extra electron is added to the 4s orbital so that order is restored and Madelung's rule applies.

[Ar] $3d^5\,4s^2$

Madelung's rule applies for the next three elements but trouble occurs again for the element copper $_{29}Cu$.

Violation 2: Madelung's rule would give the electron configuration as: [Ar] $3d^9\ 4s^2$ but the actual configuration is: [Ar] $3d^{10}\,4s^1$

So not only is the ninth electron added to the 3d orbital, another electron is "pinched" from the 4s orbital to fill the 3d shell with 10 electrons. An explanation for this is that full shells are more stable. So the copper atom arranges the electrons to make the 3d shell full.

Madelung's rule then correctly describes the electron configuration up to krypton $_{36}Kr$ which has the electron configuration: [Ar] $3d^{10}\ 4s^2\ 4p^6$
This configuration is abbreviated to [Kr].

The next two elements are correctly described by Madelung's rule. So the electron configuration of strontium $_{38}Sr$ is: [Kr] $5s^2$

Filling the 4d sub-shell

According to Madelung's rule the filling of the atomic orbitals of the next ten elements would involve adding 10 electrons, in turn, to the 4d sub-shell.

This works for the next 2 elements up to zirconium $_{40}Zr$ which has the electron configuration: [Kr] $4d^2\ 5s^2$ but then things go awry.

Madelung's rule breaks down, for the third time, for element chromium $_{41}Nb$.

Violation 3: Madelung's rule would give the electron configuration as: [Kr] $4d^3\ 5s^2$ but the actual configuration is: [Kr] $4d^4\,5s^1$

So not only is the third electron added to the 4d orbital, another electron is "pinched" from the 5s orbital to give 4 electrons in the 4d shell.
This time a half-shell is not completed.

The electron configuration of the next element, molybdenum $_{42}Mb$, also violates Madelung's rule.

Violation 4: Madelung's rule would give the electron configuration as: [Kr] $4d^4\ 5s^2$ but the actual configuration is: [Kr] $4d^5\,4s^1$

So rather than the extra electron filling-up the 5s sub-shell, it completes the 4d half-shell instead.

The electron configuration of the next element technetium $_{43}Tc$, is correctly described by Madelung's rule; [Kr] $4d^5\,4s^2$

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Filling the 4d sub-shell: Continued …

For the next element, ruthenium $_{44}$ Ru, according to Madelung's rule the added electron would be the sixth in the sub-shell 4d.

Violation 5: Madelung's rule would give the electron configuration as: [Kr] $4d^6\ 5s^2$ but the actual configuration is: [Kr] $4d^7\ 5s^1$

So not only is the sixth electron added to the 4d orbital, another electron is "pinched" from the 5s orbital to give 7 electrons in the 4d shell.
This violation does not involve a half-shell being completed.

Violation 6: The electron configuration of the next element, rhodium $_{45}$ Rh, also violates Madelung's rule because although the seventh extra electron is added to the 4d sub-shell the 5s sub-shell remains unfilled.

The electron configuration of rhodium $_{45}$ Rh is: [Kr] $4d^8\ 5s^1$

The next breakdown of Madelung's rule is probably the most interesting case of all.

Violation 7: According to Madelung's rule, the electron configuration of the next element, palladium $_{46}$ Pd, would be: [Kr] $4d^8\ 5s^2$.
However, starting from the configuration of rhodium, not only is the eighth extra electron added to the 4d sub-shell but also the remaining electron in the 5s sub-shell is "pinched" to complete the 4d sub-shell.

So the electron configuration of palladium $_{46}$ Pd is: [Kr] $4d^{10}$

Consequently, all sub-shells up to and including 4d are full but there are no electrons in the 5s sub-shell.

The next two elements involve the filling of the 5s sub-shell.

Violation 8: According to Madelung's rule, the electron configuration of the next element, silver $_{47}$ Ag, would be: [Kr] $4d^9\ 5s^2$.

However, the ninth extra electron goes on its own in the 5s sub-shell to give the configuration: [Kr] $4d^{10}\ 5s^1$.

For the next element, cadmium $_{48}$ Cd, the tenth extra electron completes the 5s sub-shell so that the electron configuration is correctly described by Madelung's rule.

The configuration of cadmium is: [Kr] $4d^{10}\ 5s^2$.

Madelung's rule then correctly describes the electron configuration for the next six elements up to xenon $_{54}$Xe which has the electron configuration:
[Kr] $4d^{10}\ 5s^2\ 5p^6$ This configuration is abbreviated to [Xe].

The next two elements are correctly described by Madelung's rule. So the electron configuration of barium $_{56}$Ba is: [Xe] $6s^2$

Now it is time to consider the lanthanum series: lanthanum $_{57}$La to lutetium $_{71}$Lu.

Despite the turmoil of the previous row of transition metals, only 3 elements in the lanthanum series violate Madelung's rule.

Filling the 4f sub-shell

According to Madelung's rule, starting with the electron configuration for barium, the next 14 electrons would be added, in turn, to the 4f sub-shell.

Violation 9: Ominously, things go wrong straight away because the first extra electron gets added to the 5d sub-shell rather than the 4f sub-shell.
So the electron configuration of lanthanum is: [Xe] $5d^1\ 6s^2$

Violation 10: For the next element, cerium $_{58}$Ce, Madelung's rule gives the electron configuration as: [Xe] $4f^2\ 6s^2$
However, although the second extra electron goes into the 4f sub-shell, there is still an electron in the 5d sub-shell.
The actual electron configuration of cerium is: [Xe] $4f^1\ 5d^1\ 6s^2$

It is worth highlighting the electron configuration of the next element, praseodymium $_{59}$Pr which is correctly described by Madelung's rule.
Not only is the third extra electron added to the 4f sub-shell, the electron which was in the 5d sub-shell is "pinched" by the 4f sub-shell to give the configuration [Xe] $4f^3\ 6s^2$

Madelung's rule also correctly describes the electron configuration of the next 4 elements up to and including europium $_{63}$Eu which has the configuration [Xe] $4f^7\ 6s^2$.

Violation 11: According to Madelung's rule, the electron configuration of the next element, gadolinium $_{64}$Gd, would be: [Xe] $4f^8\ 6s^2$.
However, rather than being added to the 4f sub-shell , the eighth extra electron goes into the 5d sub-shell instead.
So the actual electron configuration of gadolinium is: [Xe] $4f^7\ 5d^1\ 6s^2$

The electron configuration of the next element, terbium $_{65}$Tb is correctly described by Madelung's rule.
Not only is the ninth extra electron added to the 4f sub-shell, the electron which was in the 5d sub-shell is "pinched back" by the 4f sub-shell to give the configuration [Xe] $4f^9\ 6s^2$.

The final five extra electrons are added, in turn, to the 4f sub-shell so that the electron configuration of ytterbium $_{70}$Yb is: [Xe] $4f^{14}\ 6s^2$.

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Filling the 5d sub-shell

According to Madelung's rule the next 10 extra electrons will be added, in turn, to the 5d sub-shell.

The next element, lutetium $_{71}$Lu, which is the final element of the lanthanum series, has the expected electron configuration: [Xe] $4f^{14}\,5d^{1}\,6s^{2}$.

The next six elements up to and including iridium $_{77}$Ir are correctly described by Madelung's rule. So the electron configuration of iridium $_{77}$Ir is: [Xe] $4f^{14}\,5d^{7}\,6s^{2}$.

Violation 12: According to Madelung's rule, the electron configuration of the next element, platinum $_{78}$Pt, would be: [Xe] $4f^{14}\,5d^{8}\,6s^{2}$.
Although the eighth extra electron is added to the 5d sub-shell as required, another electron from the 6s sub-shell is "pinched" by the 5d sub-shell.
So the actual electron configuration of platinum is: [Xe] $4f^{14}\,5d^{9}\,6s^{1}$

Violation 13: According to Madelung's rule, the electron configuration of the next element, gold $_{79}$Au, would be: [Xe] $4f^{14}\,5d^{9}\,6s^{2}$.
Although the ninth extra electron is added to the 5d sub-shell, there is still an extra electron in this 5d sub-shell which has been "pinched" from the 6s sub-shell.
So the actual electron configuration of gold is: [Xe] $4f^{14}\,5d^{10}\,6s^{1}$

For the next element, mercury $_{80}$Hg, the tenth extra electron completes the 6s sub-shell so that the electron configuration is correctly described by Madelung's rule.

The configuration of mercury is: [Xe] $4f^{14}\,5d^{10}\,6s^{2}$.

Madelung's rule then correctly describes the electron configuration for the next six elements up to radon $_{86}$Rn which has the electron configuration: [Xe] $4f^{14}\,5d^{10}\,6s^{2}\,6p^{6}$ This configuration is abbreviated to [Rn].

The next two elements are correctly described by Madelung's rule. So the electron configuration of radium $_{88}$Ra is: [Rn] $7s^{2}$

Now it is time to consider the actinium series: actinium $_{89}$Ac to lawrencium $_{103}$Lr.

Although 88 elements have been considered so far, only 13 of the 22 violations of Madelung's rule have arisen.

Things change drastically since the electron configuration of the first five elements in the actinium series violate Madelung's rule.

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Filling the 5f sub-shell

According to Madelung's rule the next 14 extra electrons will be added, in turn, to the 5f sub-shell.

Violation 14: According to Madelung's rule, the electron configuration of the next element, actinium 89 Ac, would be: [Rn] $5f^1$ $7s^2$.
However, rather than being added to the 5f sub-shell , the first extra electron goes into the 6d sub-shell instead.
So the actual electron configuration of actinium is: [Rn] $6d^1$ $7s^2$

Violation 15: For the next element, thorium 90 Th, Madelung's rule gives the electron configuration as: [Rn] $5f^2$ $7s^2$.
However, the second extra electron also goes into the sub-level 6d rather than the 5f sub-level .
So the actual electron configuration of thorium is: [Rn] $6d^2$ $7s^2$

Violation 16: For the next element, protactinium 91 Pa, Madelung's rule gives the electron configuration as: [Rn] $5f^3$ $7s^2$.
Although the third extra electron is added to the 5f sub-shell and one of the electrons in the 6d sub-shell is "pinched" by the 5f sub-shell there is still one electron in the 6d shell.
So the actual electron configuration of protactinium is: [Rn] $5f^2$ $6d^1$ $7s^2$

Violation 17: For the next element, uranium 92 U, Madelung's rule gives the electron configuration as: [Rn] $5f^4$ $7s^2$.
Although the fourth extra electron is added to the 5f sub-shell there is still one electron in the 6d shell.
So the actual electron configuration of uranium is: [Rn] $5f^3$ $6d^1$ $7s^2$

Violation 18: For the next element, neptunium 93 Np, Madelung's rule gives the electron configuration as: [Rn] $5f^5$ $7s^2$.
Although the fifth extra electron is added to the 5f sub-shell there is still one electron in the 6d shell.
So the actual electron configuration of neptunium is: [Rn] $5f^4$ $6d^1$ $7s^2$

The electron configuration of the next element, plutonium 94 Pu is correctly described by Madelung's rule.
Not only is the sixth extra electron added to the 5f sub-shell, the electron which was in the 6d sub-shell is "pinched back" by the 5f sub-shell to give the configuration [Rn] $5f^6$ $7s^2$.

The electron configuration of the next element, americium 95 Am, is correctly described by Madelung's rule: [Rn] $5f^7$ $7s^2$.

Violation 19: According to Madelung's rule, the electron configuration of the next element, curium 96 Cm, would be: [Rn] $5f^8$ $7s^2$.
However, rather than being added to the 5f sub-shell , the eighth extra electron goes into the 6d sub-shell instead.
So the actual electron configuration of curium is: [Rn] $5f^7$ $6d^1$ $7s^2$

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Filling the 5f sub-shell: Continued …

The electron configuration of the next element, berkelium 97 Bk is correctly described by Madelung's rule.
Not only is the ninth extra electron added to the 5f sub-shell, the electron which was in the 6d sub-shell is "pinched back" by the 5f sub-shell to give the configuration [Rn] $5f^9$ $7s^2$.

The final five extra electrons are added, in turn, to the 5f sub-shell so that the electron configuration of nobelium 102 No is: [Rn] $5f^{14}$ $7s^2$.

Filling the 6d sub-shell:

According to Madelung's rule the next 10 extra electrons will be added, in turn, to the 6d sub-shell.

Violation 20: According to Madelung's rule, the electron configuration of the next element, lawrencium 103 Lr (which is the final element of the actinium series) would be: [Rn] $5f^{14}$ $6d^1$ $7s^2$.
However, the extra electron is added to the 7p sub-shell rather than the 6d sub-shell.
So the actual electron configuration of lawrencium is: [Rn] $5f^{14}$ $7s^2$ $7p^1$

The electron configuration of the next element, rutherfordium 104 Rf is correctly described by Madelung's rule.
Not only is the second extra electron added to the 6d sub-shell, the electron which was in the 7p sub-shell is "pinched back" by the 6d sub-shell to give the configuration [Rn] $5f^{14}$ $6d^2$ $7s^2$.

The next 5 elements up to and including meitnerium 109 Mt are correctly described by Madelung's rule.

So the electron configuration of meitnerium 109 Mt is: [Rn] $5f^{14}$ $6d^7$ $7s^2$.

Violation 21: For the next element, darmstadtium 110 Ds, Madelung's rule gives the electron configuration as: [Rn] $5f^{14}$ $6d^8$ $7s^2$.
However, although the eighth extra electron goes into the sub-level 6d, one of the electrons in the 7s sub-level is "pinched" by the 6d sub-level.
So the actual electron configuration of darmstadtium is: [Rn] $5f^{14}$ $6d^9$ $7s^1$.

Violation 22: For the next element, roentgenium 111 Rg, Madelung's rule gives the electron configuration as: [Rn] $5f^{14}$ $6d^9$ $7s^2$.
Although the ninth extra electron is added to the 6d sub-shell, there is still an extra electron in this 6d sub-shell which has been "pinched" from the 7s sub-shell.
So the actual electron configuration of roentgenium is: [Rn] $5f^{14}$ $6d^{10}$ $7s^1$.

For the next element, copernicium 112 Cn, the tenth extra electron completes the 7s sub-shell so that the electron configuration is correctly described by Madelung's rule. The configuration of copernicium is: [Rn] $5f^{14}$ $6d^{10}$ $7s^2$.

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Filling the 7p sub-shell:

The six extra electrons are added, in turn, to the 7p sub-shell in accordance with Madelung's rule up to and including the element oganesson.

The heaviest element known so far is: oganesson $_{118}$Og which has the electron configuration: [Rn] $5f^{14}$ $6d^{10}$ $7s^{2}$ $7p^{6}$.

A summary of the 22 violations of Madelung's rule is shown in the file: Madelung Rule Violations.

The periodic table in which elements that violate the Madelung rule are highlighted is shown in the file: Periodic Table.

ATOMIC PICTURES

An atomic picture displays the number of protons and neutrons in the nucleus and the number of electrons in the electron shells.

For example, given that the electron configuration of gold $^{197}_{79}$Au is [Xe] $4f^{14}$ $5d^{10}$ $6s^{1}$, draw the atomic picture for gold.

Since the nucleon number is 197 and there are 79 protons in the nucleus of the gold atom, the number of neutrons = 197 - 79 = 118.

The electron configuration of Xenon is: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ $4s^2$ $4p^6$ $4d^{10}$ $5s^2$ $5p^6$

So the electron configuration of gold is: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $3d^{10}$ $4s^2$ $4p^6$ $4d^{10}$ $5s^2$ $5p^6$ $4f^{14}$ $5d^{10}$ $6s^1$

Count the number of electrons in the electron shells (depicted by n).

Number of electrons in the n = 1 shell: 2
Number of electrons in the n = 2 shell: 2 + 6 = 8
Number of electrons in the n = 3 shell: 2 + 6 + 10 = 18
Number of electrons in the n = 4 shell: 2 + 6 + 10 + 14 = 32
Number of electrons in the n = 5 shell: 2 + 6 + 10 = 18
Number of electrons in the n = 6 shell: 1

Check: 2 + 8 + 18 + 32 + 18 + 1 = 79 (as required).

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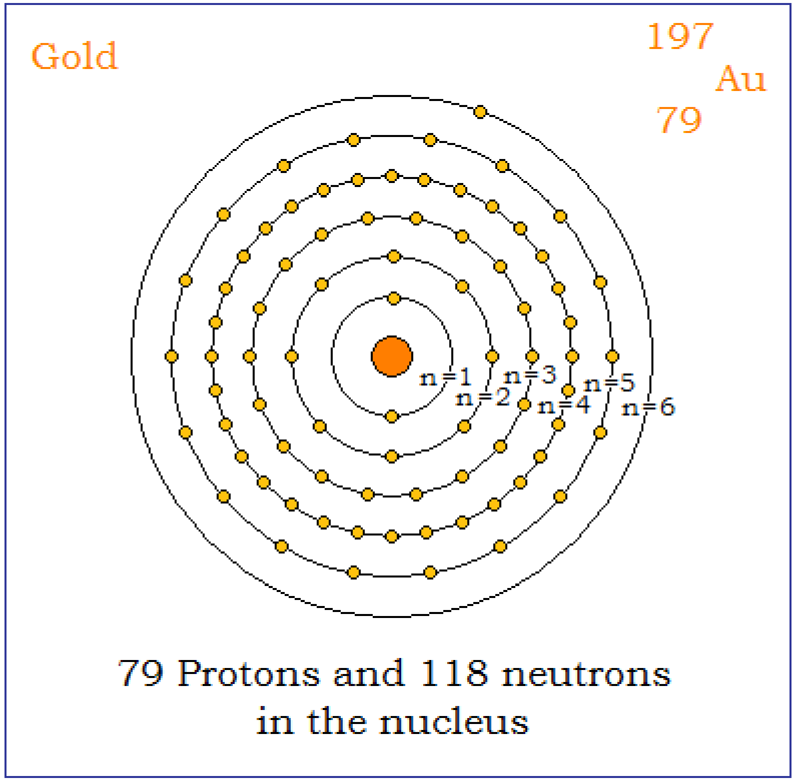
The Atomic Picture of Gold



The number of electrons in the electron shells for gold are: 2, 8, 18, 32, 18, 1