3.5

3.

Table 3 Sommerfeld's Electron Energy Sublevels

Primary energy level	Principal quantum number, n	Possible secondary quantum numbers, l	Number of sublevels per primary level
1	1	0	1
2	2	0,1	4
3	3	0,1,2	9
4	4	0,1,2,3	16

4. For any principal quantum number, n, the highest possible value of l is $n–1$.
5. For any principal quantum number, n, the possible values of l include all of the integers from 0 to $n–1$.

SECTION 3.5 QUESTIONS

(Page 184)

Understanding Concepts

1. The main kind of evidence used comes from atomic line spectra, particularly the splitting of lines.
2. The first quantum number describes the main energy level; the second quantum number describes small energy level steps within the main energy level corresponding to different shapes of "orbits"; the third quantum number describes the orientation in space of the electron "orbits"; and the fourth quantum number describes the "spin" of electrons.
3. (a) For $l = 0$, 1, 2, and 3, there are 0, 3, 5, and 7 possible values of m_l, respectively.
   (b) Each number is the next greater odd integer (or $2l + 1$ for all ls except $l = 0$).
   (c) From the answer to (b), the number of possible values for m_l for $l = 4$ must be 9 (the next odd integer).
4. The fourth quantum number is m_s, and it is necessary to explain magnetic properties of atoms.
5.

Table 4 Summary of Quantum Numbers

(n)	(0 to n – 1)	(–l to +l)	(+1/2 or –1/2)
4	0	0	+1/2, –1/2
	1	-1, 0, +1	+1/2, –1/2
	2	-2, -1, 0, +1, +2	+1/2, –1/2
	3	-3, -2, -1, 0, +1, +2, +3	+1/2, –1/2

6. It takes four quantum numbers to describe fully an electron in an atom. An example listing labels and values of each quantum number might be $n = 2$, $l = 1$, $m_l = –1$, and $m_s = +1/2$. This might describe an electron in a hydrogen atom in an "excited" state.
7. For each principal quantum number from $n = 1$ to $n = 3$ (see Table 4), there can be 2, 8, and 18 different electron descriptions.
8. In the development of scientific knowledge, empirical knowledge usually comes first. Examples from this section are the investigation of bright line spectra and of magnetic effects upon these spectra—both of which preceded the theory that attempts to explain them in terms of atomic structure.

3.6 ATOMIC STRUCTURE AND THE PERIODIC TABLE

PRACTICE

(Page 191)

Understanding Concepts

1. The aufbau principle states that electrons occupy lowest energy orbitals first. The Pauli exclusion principle states that no more than two electrons (of opposite spin) may occupy the same orbital, and Hund's rule states that electrons are not paired within sublevel orbitals until each sublevel orbital has at least one electron.

2. A periodic table can be used to help complete energy level diagrams because it is arranged according to electron energy levels, sublevels, and orbitals.

3. (a) 3p ↑ ↑ ↑
3s ↑↓
2p ↑↓ ↑↓ ↑↓
2s ↑↓
1s ↑↓
phosphorus atom, P

(b) 4s ↑
3p ↑↓ ↑↓ ↑↓
3s ↑↓
2p ↑↓ ↑↓ ↑↓
2s ↑↓
1s ↑↓
potassium atom, K

(c) 3d ↑ ↑ ↑ ↑ ↑
4s ↑↓
3p ↑↓ ↑↓ ↑↓
3s ↑↓
2p ↑↓ ↑↓ ↑↓
2s ↑↓
1s ↑↓
manganese atom, Mn

(d) 2p ↑↓ ↑↓ ↑↓
2s ↑↓
1s ↑↓
nitride ion, N^{3-}

(e) 4p ↑↓ ↑↓ ↑↓
3d ↑↓ ↑↓ ↑↓ ↑↓ ↑↓
4s ↑↓
3p ↑↓ ↑↓ ↑↓
3s ↑↓
2p ↑↓ ↑↓ ↑↓
2s ↑↓
1s ↑↓
bromide ion, Br^-

(f)

4d ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

5s __

4p ↑↓ ↑↓ ↑↓

3d ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

4s ↑↓

3p ↑↓ ↑↓ ↑↓

3s ↑↓

2p ↑↓ ↑↓ ↑↓

2s ↑↓

1s ↑↓

cadmium ion, Cd^{2+}

4. (a)

3p ↑↓ ↑↓ ↑↓	3p ↑↓ ↑↓ ↑↓
3s ↑↓	3s ↑↓
2p ↑↓ ↑↓ ↑↓	2p ↑↓ ↑↓ ↑↓
2s ↑↓	2s ↑↓
1s ↑↓	1s ↑↓
potassium ion, K^+	chloride ion, Cl^-

(b) An atom of the noble gas argon, Ar, has the same electron orbital energy level diagram as do these two ions.

Extension

5. 1*s* would be $n = 1, l = 0$
   2*s* would be $n = 2, l = 0$
   2*p* would be $n = 2, l = 1$
   3*d* would be $n = 3, l = 2$

PRACTICE

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Understanding Concepts

6. (a) beryllium
   (b) fluorine
   (c) sodium
   (d) sulfur

7.	sodium	$1s^2\ 2s^2\ 2p^6 3s^1$
	magnesium	$1s^2\ 2s^2\ 2p^6 3s^2$
	aluminum	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^1$
	silicon	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^2$
	phosphorus	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^3$
	sulfur	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^4$
	chlorine	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^5$
	argon	$1s^2\ 2s^2\ 2p^6 3s^2\ 3p^6$
8.	fluorine	[He] $2s^2\ 2p^5$
	chlorine	[Ne] $3s^2\ 3p^5$
	bromine	[Ar] $4s^2\ 4p^5$ → $3d^{10}$
	iodine	[Kr] $5s^2\ 5p^5$ →
	astatine	[Xe] $6s\ 6p^5$ →

Each halogen configuration ends with two *s* and three *p* orbitals.

Other chemical families, such as the alkali metals, also have similar valence orbital configurations.

9. fluoride ion $1s^2\ 2s^2\ 2p^6$
   sodium ion $1s^2\ 2s^2\ 2p^6$
10. Isoelectronic means having the same number of electrons.
11. zinc ion [Ar] $3d^{10}$
   cadmium ion [Kr] $4d^{10}$
   mercury(II) ion [Xe] $4f^{14}\ 5d^8$

SECTION 3.6 QUESTIONS

(Page 197)

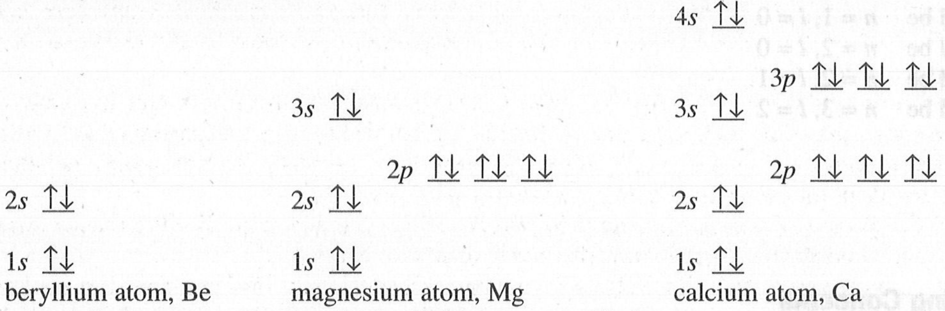
Understanding Concepts

1. Maximum number of electrons: (a) $2e^-$ (b) $8e^-$ (c) $18e^-$ (d) $32e^-$
2.

Orbitals and Electrons in *s*, *p*, *d*, and *f* Sublevels

Sublevel	Symbol	Value of *l*	Number of orbitals	Max # of electrons
(a)	*s*	0	1	2
(b)	*p*	1	4	8
(c)	*d*	2	9	18
(d)	*f*	3	16	32

3. The aufbau principle states that electrons occupy lower energy orbitals first. Either a diagonal orbital diagram or the periodic table can be used to determine this order of occupancy.
4. If four electrons are to be placed into a *p* subshell, the aufbau principle states that all lower energy levels must already be full, and Hund's rule states that each of the three *p* orbitals must already have one occupying electron before the fourth is placed in any one of the orbitals.
5. (a)



   (b) These diagrams all show two *s* electrons in the highest energy orbital.
6. (a) *s*
   (b) *d*
   (c) *p*
   (d) *f*
7. (a) The halide ions have a charge of negative one, –1.
   (b) The electron configuration of each halogen shows one less electron than a full *p* orbital energy level; for example, fluorine is $1s^2\ 2s^2\ 2p^5$, chlorine is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$, bromine is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$, and so on. We explain the ion charge by assuming that halogens strongly attract one extra electron to occupy the unfilled *p* orbital in the highest orbital energy level.
8. (a) A sodium ion, Na^+, has a configuration of $1s^2\ 2s^2\ 2p^6$, the same as that of a neon atom, Ne.
   (b) These two chemical entities are both chemically very stable, and have the same electron configuration; but sodium ions are positively charged and strongly attract negative ions to form ionic solid compounds, while neutral neon atoms have extremely weak attractive forces, and form a noble gas at room conditions.
9. The electron configuration for Sb^{3+} is [Kr] $5s^2\ 4d^{10}$. The electron configuration for Sb^{5+} is [Kr]$4d^{10}$.
10. The electron configuration for a gallium atom, Ga, is [Ar] $4s^2\ 3d^{10}\ 4p^1$. The Ga^{3+} ion has most probably lost three electrons from the fourth shell, and so should have a configuration of [Ar] $3d^{10}$.
11. Copper has an electron configuration of [Ar] $4s^1\ 3d^{10}$ and therefore has an unpaired electron ($4s^1$). Zinc has an electron configuration of [Ar] $4s^2\ 3d^{10}$ and has no unpaired electrons.

12. A gold atom should have an electron configuration of [Xe] $6s^2\ 4f^{14}\ 5d^9$, if we use the aufbau principle. However, a filled *d* suborbital creates extra stability, especially in large atoms, so [Xe] $6s^1\ 4f^{14}\ 5d^{10}$ is the normal configuration.

13. (a) Sc^{3+} has a probable configuration of $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$, or [Ar].
    (b) Ag^+ has a probable configuration of [Kr] $4d^{10}$.
    (c) Fe^{3+} has a probable configuration of [Ar] $3d^5$.
    Fe^{2+} has a probable configuration of [Ar] $4s^1\ 3d^5$.
    (d) Th^+ has a probable configuration of [Rn] $7s^2\ 5f^1$.
    Th^{3+} has a probable configuration of [Rn] $5f^1$.

14. Carbon, silicon, and germanium atoms have (respectively) electron configurations of $1s^2\ 2s^2\ 2p^2$, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$, and $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^2$. Each of these atoms has four electrons in the highest numbered shell of orbitals, and likely use these four electrons for bonding.

Applying Inquiry Skills

15. (a) The result predicted by classical theory is that the atoms should hit a target to form a solid pattern because the atoms should hit the photographic plate randomly within the beam. The result predicted by quantum theory is that the pattern should be two distinct lines.
    (b) Silver has an electron configuration of [Kr] $5s^1\ 4d^{10}$, with a single unpaired *s* valence electron. If all silver atoms were identical, any magnetic moment caused by the external field should move the atoms in random directions, since it could be oriented in any direction as the atoms enter the field. The two distinct lines indicate that a silver atom must have one of two distinct and opposite magnetic moments. This was later interpreted to be due to the valence (unpaired) electron having one of only two possible (and opposite) "spins."

Making Connections

16. (a) Dimes were shipped out of the country because it is illegal to deface or alter Canadian currency in Canada.
    (b) These metals have very different magnetic properties, which could be used to separate them.
    (c) A magnet should separate these coins easily, because nickel is ferromagnetic (strongly magnetic) and silver is not.

17. ESR spectroscopy places samples of paramagnetic material in a high uniform magnetic field to split the energy levels of the ground state. The results can be used to help determine molecular structures and properties, such as the degree of movement (rotation) of side groups on structures. Another area deals with finding probable redox activation sites on protein molecules. The dynamics (movements) of molecules in liquid and solid phases can be examined to determine properties of new materials.

18. MRI uses alterations to the spin of a proton—which has two quantum states like that of an electron—to cause signals to be emitted from materials such as human tissue that can be used to scan the interior of the material in great detail, without harmful invasion of the material by physical objects or high-energy electromagnetic radiation. Like ESR, MRI uses a very powerful magnetic field to align subatomic particles.

    MRI has its major use in medicine, where it provides excellent detailed scans of soft tissue, allowing doctors to diagnose illness and abnormalities much more effectively than with X rays.

    The political issue associated with MRI use is the cost of health care. MRI machines are very valuable to doctors, but the machines (and the technicians to run them) are in short supply, highly technical, and very expensive.

3.7 WAVE MECHANICS AND ORBITALS

SECTION 3.7 QUESTIONS

(Page 202)

Understanding Concepts

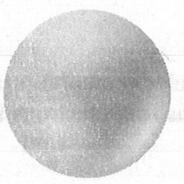
1. (a) Louis Victor, 7th Duc de Broglie, believed that particles could have properties and characteristics of waves, and that this effect would be significant for tiny, fast-moving particles like electrons.
   (b) Erwin Schrödinger imagined electron behaviour within the atom structure as a wave phenomenon, described by a wave mechanical equation.
   (c) Werner Heisenberg thought that electron behaviour cannot ever be exactly described, but only discussed as a probability system, within limits imposed by his "uncertainty principle."

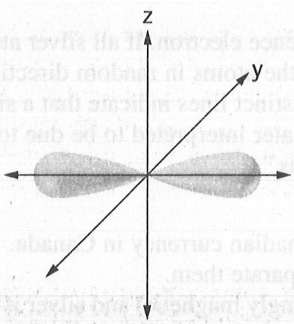
2. An electron orbital describes the three-dimensional region of space occupied by an electron, that is, in which we calculate a high probability (usually > 90%) of detecting an electron of a specific energy.

   An orbit is a simplified (incorrect, but useful) idea describing electrons as orbiting nuclei in circular or elliptical paths.

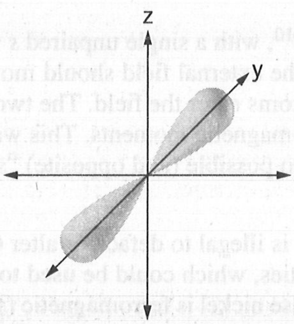
3. Quantum mechanics provides both the general shape (volume of space), and the electron probability density, within an orbital.
4. Quantum mechanics theory says nothing about either the position or about the motion of an electron within an orbital.
5. The 1*s* and 2*s* orbitals are spherical in shape, with the 2*s* orbital considerably larger and having two concentric regions of high probability density. A 2*p* orbital is shaped like a dumbbell, with two areas of high probable density, one on each side of the nucleus.


1*s*

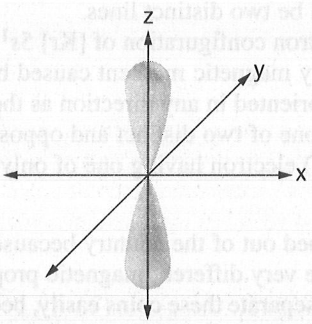

2*s*



$2p_x$



$2p_y$



$2p_z$

Making Connections

6. Statistics are used to predict situations such as the number of megajoules of electricity that will be used in a city in a given winter month, or the number of students that will achieve honours on a national examination, or the number of cases of influenza that will occur over the winter in a country. All statistical prediction is based on probability, meaning it always includes some uncertainty, and predicts better for larger samples and longer times—as does quantum mechanics.
7. Heisenberg would argue that the measured speed included uncertainty; but the amount of this uncertainty is infinitesimal for an object such as a car, certainly many orders of magnitude less than the precision of the "radar" gun.
8. Dr. Richard Bader researches the nature of atoms and bonds within molecular structures, attempting to achieve a level of understanding that will allow predictions of the properties of materials to be made by theory using computer calculations. His theory of molecular topologies is directly related to the quantum mechanics of atoms—the constituents of the structures with which he deals.
9. Areas where superconductivity is presently used include creating the very strong magnetic fields for MRI scanning (superconducting electromagnets), for magnetic shielding devices, infrared sensors, microwave signal devices, and quantum interference devices. Some projected uses are for "maglev" high-speed trains and ships, power generation and transmission, energy storage systems, high-speed particle accelerators, and precision magnetic separation devices.
10. The highest temperature at which superconductivity has been achieved is > 130 K. The substance used is a metal oxide composite (a material that has properties of a ceramic), one of a general class called *peroskovites.* These substances have formulas such as $YBa_2Cu_3O_{7(s)}$, the famous 1-2-3 oxide of yttrium, barium, and copper, which was the first material to superconduct at a temperature higher than that of boiling liquid nitrogen (–196 °C or 77 K).

3.8 APPLICATIONS OF QUANTUM MECHANICS

Try This Activity: Bar Code Scanners

(Page 205)

(a) Red or white areas reflect red laser light strongly; black, dark blue, and green areas least strongly.

(b) Bar code scanners read the bright-to-dark-to-bright light level changes, and how long they last (which depends on the code line width) as an information signal.

SECTION 3.8 QUESTIONS

(Page 206)

Understanding Concepts

1. Laser light is *monochromatic* (one colour/wavelength/frequency), *coherent* (acts like one long continuous wave), and *collimated* (rays are quite precisely parallel).
2. Lasers work on a principle of raising many electrons to a higher energy level, and then stimulating them to drop to a lower level all at once, producing an output of a very large number of photons.
3. Applications of the principles of quantum mechanics in medical diagnosis include the use of infrared spectroscopes to detect traces of substances in body tissues and fluids; and the use of MRI machines to scan the inside of the body by causing tissues to emit microwave radiation.

Making Connections

4. (Student reports will vary, but should include a basic description and diagrams of X-ray diffraction due to interference of the very short electromagnetic wavelengths with the similarly sized spacings between entities in solid crystals—which provides information about the sizes, shapes, charges, and arrangements of these entities in condensed phases. A simple parallel phenomenon is the diffraction pattern created when a pocket laser pointer beam is reflected from the surface of a CD. The angular displacement of the secondary images is proportional to the line spacing on the CD. Students with physics background in calculations of the diffraction of light from diffraction gratings can easily calculate the CD line spacing using the same technique.)

CAREERS IN CHEMISTRY

PRACTICE

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Making Connections

1. (A typical report would include information such as:)
   In the field of Biochemistry, a gene medicine scientist may do precise mass determinations of purified peptides, proteins, and oligosaccharides, using MALDI (Matrix Assisted Laser Desorption/Ionization time of flight) mass spectroscopic analysis. A scientist in charge of this area for a company would also prepare complex biological samples and determine atomic sequencing in organic molecules, in order to identify and develop new therapeutic materials. Such a position would require a Ph.D. in biochemistry or chemistry, preferably with a few years postdoctoral experience, or an M.Sc. in biochemistry with 10+ years of related experience. People in this area are in demand worldwide, and annual salaries on the order of $100 000 are not uncommon in industrial areas.

CHAPTER 3 LAB ACTIVITIES

INVESTIGATION 3.1.1 THE NATURE OF CATHODE RAYS

(Page 209)

Evidence/Analysis

(a)

Observations of a Cathode Ray and Laser Light

	Cathode ray	Laser light
Effect of bar magnet	ray moves perpendicular to the long axis of bar magnet	no effect
Effect of charged plates	ray moves toward positive plate and away from negative plate	no effect

(b) According to the evidence collected, both electric charges and magnets change the direction of cathode rays but not laser light. Therefore, cathode rays are different in nature from electromagnetic radiation like visible light.

Evaluation

(c) There are no obvious flaws in the design. The materials and procedure could be improved by including several different sources of cathode rays and different types of light. This would produce more evidence to make the answer to the question more certain.
(Other effects could also be tested.)

(d) The hypothesis that cathode rays are a form of electromagnetic radiation has been shown to be false because the evidence clearly shows significant differences between cathode rays and light.

Synthesis

(e) The bending of cathode rays when passing near electrically charged plates suggests that cathode rays contain charged particles.

(f) Opposite electric charges attract each other and like charges repel. The evidence that cathode rays are attracted to the positively charged plate and repelled from the negative plate suggests that cathode rays contain negatively charged particles.

ACTIVITY 3.1.1 RUTHERFORD'S GOLD FOIL EXPERIMENT

(Page 210)

- animation mode; activity of source = average; scintillations set to remain; time = 5 min
- Most alpha particles are deflected within 20° of the straight-line path; a few alpha particles are deflected up to 40°, occasionally up to 60°, and very rarely beyond 90° (only 2 in this simulation).

(a) According to the Thomson atom model, a stream of alpha particles should pass more or less straight through a gold foil, perhaps deflecting a little.

(b) Rutherford's results showed that the majority of alpha particles deflected little but some alpha particles deflected significantly and few appeared to "bounce back."

(c) Almost all of the alpha particles were relatively undeflected, suggesting that the nucleus is very much smaller than the atom, because most alpha particles miss it completely.

(d) The evidence conflicts strongly with the Thomson model, which therefore must be replaced with a new model.

(e) The general pattern of the results with aluminum foil should be similar to that with the gold foil. With aluminum foil, fewer alpha particles should deflect through significant angles because an aluminum nucleus (13 p^+) is not as positive as a gold nucleus (79 p^+).

ACTIVITY 3.3.1 HOT SOLIDS

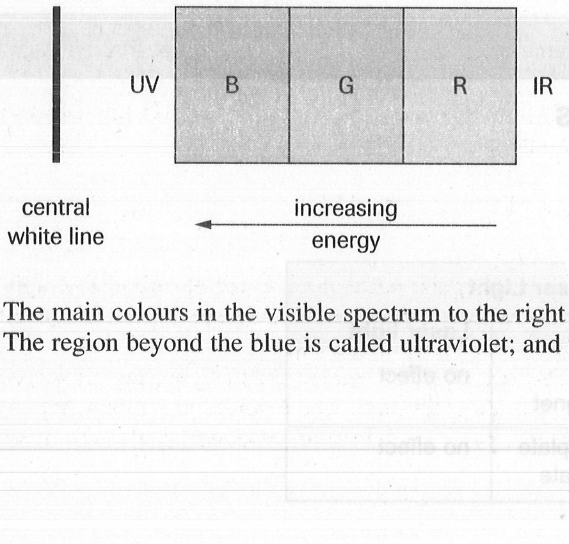
(Page 210)

(a) The filament starts with a dim, orange-red colour that becomes brighter and more orange, and then brighter and more yellow, and then brighter still and white.

(b) "White hot" objects are much hotter than "red hot" ones.

(c) Objects in a home that may be red hot at certain times include electric stove elements and wires in electric toasters.

(d)



The main colours in the visible spectrum to the right of the central white line are blue, green, and red.

(e) The region beyond the blue is called ultraviolet; and the region beyond the red is called infrared.