Chapter 3

Molecules, Compounds, and
Chemical Composition
Elements and Compounds

Elements combine together to make an almost limitless number of compounds.

The properties of the compound are totally different from the constituent elements.

<table>
<thead>
<tr>
<th>Selected Properties</th>
<th>Hydrogen</th>
<th>Oxygen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boiling Point</td>
<td>–253 °C</td>
<td>–183 °C</td>
</tr>
<tr>
<td>State at Room Temperature</td>
<td>Gas</td>
<td>Gas</td>
</tr>
<tr>
<td>Flammability</td>
<td>Explosive</td>
<td>Necessary for combustion</td>
</tr>
</tbody>
</table>

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Mixtures and Compounds

Hydrogen and Oxygen Mixture
Can have any ratio of hydrogen to oxygen.

Water (A Compound)
Water molecules have a fixed ratio of hydrogen (2 atoms) to oxygen (1 atom).
Chemical Bonds

Compounds are made of atoms held together by bonds. Chemical bonds are forces of attraction between atoms. The bonding attraction comes from attractions between protons and electrons.
**Bond Types**

Two general types of bonding between atoms found in compounds, **ionic** and **covalent**.

**Ionic bonds** result when electrons have been transferred between atoms, resulting in oppositely charged ions that attract each other.

Generally found when metal atoms bond to nonmetal atoms

**Covalent bonds** result when two atoms share some of their electrons.

Generally found when nonmetal atoms bond together
Formation of an Ionic Compound

Neutral Atoms Undergo Electron Transfer

Charged Ions

An Orderly Aggregate Called an Ionic Crystal
Formation of an Covalent Compound

Attractive

Repulsive

Electron cloud

Nucleus
Formation of a Covalent Compound

- HH (too close)
- H-H
- H········H (too far)

Energy vs. Bond length (74 pm) vs. Internuclear distance
Representative Covalent Compounds

Water, $\text{H}_2\text{O}$
Oxygen bonds to 2 hydrogen atoms.

Ammonia, $\text{NH}_3$
Nitrogen bonds to 3 hydrogen atoms.

Methane, $\text{CH}_4$
Carbon bonds to 4 hydrogen atoms.
A **compound** is a distinct substance that is composed of atoms of two or more elements.

We describe the compound by describing the number and type of each atom in the simplest unit of the compound.

Each element is represented by its letter symbol.

The number of atoms of each element is written to the right of the element as a subscript.

Polyatomic ions are placed in parentheses. (if more than one is present)
An empirical formula gives the relative number of atoms of each element in a compound.

It does not describe how many atoms, the order of attachment, or the shape.

For example:

1) The empirical formula for the ionic compound fluorspar is $\text{CaCl}_2$. This means that there is 1 Ca$^{2+}$ ion for every 2 Cl$^{-}$ ions in the compound.

2) The empirical formula for the molecular compound oxalic acid is $\text{CHO}_2$. This means that there is 1 C atom and 1 H atom for every 2 O atoms in the molecule.
Types of Formula: Molecular Formula

A molecular formula gives the actual number of atoms of each element in a molecule of a compound.

*It does not describe the order of attachment, or the shape.*

The empirical formula for the molecular compound oxalic acid is CHO$_2$.

The actual molecular formula is C$_2$H$_2$O$_4$
Types of Formula: Structural Formula

A **structural formula** uses lines to represent covalent bonds and shows how atoms in a molecule are connected or bonded to each other.

**Structural Formulas of Oxalic Acid**

\[ \text{H-O-C} \quad \text{C} \quad \text{O} \quad \text{H} \]
Molecular Models

CH₄

Molecular formula

H—C—H

H

Structural formula

Ball-and-stick model

Space-filling model
Practice — Find the empirical formula for each of the following

The ionic compound that has two aluminum ions for every three oxide ions: $\text{Al}_2\text{O}_3$

arabinose, $\text{C}_5\text{H}_{10}\text{O}_5$

pyrimidine

ethylene glycol $\text{CH}_2\text{O}$
Classifying Elements & Compounds

Atomic elements
elements whose particles are single atoms

Molecular elements
elements whose particles are multi-atom molecules

Molecular compounds
compounds whose particles are molecules

Ionic compounds
compounds whose particles are cations and anions
Molecular View of Elements and Compounds

Pure substances

- Elements
  - Atomic
    - Example: Ne
  - Molecular
    - Example: O₂

- Compounds
  - Molecular
    - Example: H₂O
  - Ionic
    - Example: NaCl
MOST ELEMENTS
Single atoms are the constituent particles. The atoms may be physically attracted to each other, but are not chemically bonded together.

A FEW ELEMENTS
Molecules are the constituent particles. The molecules are made of two or more atoms chemically bonded together by covalent bonds.
## Molecular Elements

<table>
<thead>
<tr>
<th>Periods</th>
<th>1A</th>
<th>2A</th>
<th>3A</th>
<th>4A</th>
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<td>Rf</td>
<td>Db</td>
<td>Sg</td>
<td>Bh</td>
<td>Hs</td>
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</tbody>
</table>

- Elements that exist as diatomic molecules:
- Elements that exist as polyatomic molecules

**Lanthanides**

<table>
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<tr>
<th>58</th>
<th>59</th>
<th>60</th>
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<td>Nd</td>
<td>Pm</td>
<td>Sm</td>
<td>Eu</td>
<td>Gd</td>
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**Actinides**

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<th>92</th>
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<tbody>
<tr>
<td>Th</td>
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<td>U</td>
<td>Np</td>
<td>Pu</td>
<td>Am</td>
<td>Cm</td>
<td>Bk</td>
<td>Cf</td>
</tr>
</tbody>
</table>

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Compounds

SOME COMPOUNDS
Composed of ions arranged in a 3-dimensional pattern
These are called **ionic compounds**.

OTHER COMPOUNDS
Composed of individual molecule units
Each molecule contains atoms of different elements chemically attached by covalent bonds
These are called **molecular compounds**.
Ionic vs. Molecular Compounds

A Molecular Compound

Propane – contains individual $\text{C}_3\text{H}_8$ molecules

An Ionic Compound

Table salt – contains an array of $\text{Na}^+$ ions and $\text{Cl}^-$ ions
Classify Each of the Following as Either an **Atomic Element**, **Molecular Element**, **Molecular Compound**, or **Ionic Compound**

Aluminum, Al *atomic element*
Aluminum chloride, AlCl₃ *ionic compound*
Chlorine, Cl₂ *molecular element*
Acetone, C₃H₆O *molecular compound*
Carbon monoxide, CO *molecular compound*
Cobalt, Co *atomic element*
Formula Units vs. Molecules

One formula unit

Ionic compound

One molecule

Molecular compound
Compound must have no total charge, therefore we must balance the numbers of cations and anions in a compound to get 0 charge.

**Practice — What are the formulas for compounds made from the following ions?**

<table>
<thead>
<tr>
<th>Cation</th>
<th>Anion</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Potassium ion</td>
<td>Nitride ion</td>
<td>K&lt;sup&gt;+&lt;/sup&gt; with N&lt;sup&gt;3-&lt;/sup&gt; K&lt;sub&gt;3&lt;/sub&gt;N</td>
</tr>
<tr>
<td>Calcium ion</td>
<td>Bromide ion</td>
<td>Ca&lt;sup&gt;2+&lt;/sup&gt; with Br&lt;sup&gt;-&lt;/sup&gt; CaBr&lt;sub&gt;2&lt;/sub&gt;</td>
</tr>
<tr>
<td>Aluminum ion</td>
<td>Sulfide ion</td>
<td>Al&lt;sup&gt;3+&lt;/sup&gt; with S&lt;sup&gt;2-&lt;/sup&gt; Al&lt;sub&gt;2&lt;/sub&gt;S&lt;sub&gt;3&lt;/sub&gt;</td>
</tr>
</tbody>
</table>

**Potassium nitride**

**Calcium bromide**

**Aluminum sulfide**
Formula Mass

The mass of an individual molecule or formula unit
Also known as *molecular mass* or *molecular weight*

Sum of the masses of the atoms in a single molecule or
formula unit

mass of 1 molecule of $\text{H}_2\text{O}$
$= 2(1.01 \text{ amu H}) + 16.00 \text{ amu O} = 18.02 \text{ amu}$

mass of 1 formula unit of $\text{MgCl}_2$
$= 2(35.45 \text{ amu Cl}) + 24.30 \text{ amu Mg} = 95.20 \text{ amu}$
Molar Mass
The relative masses of molecules can be calculated from atomic masses.

**Formula Mass**

\[ \text{Formula Mass} = 1 \text{ molecule of } \text{H}_2\text{O} \]
\[ = 2(1.01 \text{ amu H}) + 16.00 \text{ amu O} = 18.02 \text{ amu} \]

1 mole of \text{H}_2\text{O} contains 2 moles of H and 1 mole of O.

**Molar Mass**

\[ \text{molar mass} = 1 \text{ mole } \text{H}_2\text{O} \]
\[ = 2(1.01 \text{ g H}) + 16.00 \text{ g O} = 18.02 \text{ g} \]

so the Molar Mass of \text{H}_2\text{O} is 18.02 g/mole
**Practice — How many moles are in 50.0 g of \( \text{PbO}_2 \)? \((\text{Pb} = 207.2, \text{O} = 16.00)\)**

\[
\begin{align*}
\text{Pb} &= 1 \times 207.2 = 207.2 \\
\text{O} &= 2 \times 16.00 = 32.00 \\
\frac{\text{PbO}_2}{239.2 \text{ g/mol}} &= \frac{1 \text{ mol PbO}_2}{239.2 \text{ g}} \\
50.0 \text{ g PbO}_2 \times \frac{1 \text{ mol}}{239.2 \text{ g}} &= 0.209903 \text{ mol} = 0.209 \text{ mol PbO}_2
\end{align*}
\]
Example: Find the number of CO\(_2\) molecules in 10.8 g of dry ice

\[
1 \text{ mol CO}_2 = 44.01 \text{ g}, \quad 1 \text{ mol} = 6.022 \times 10^{23}
\]

\[
10.8 \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \times \frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol}} = 1.48 \times 10^{23} \text{ molecules CO}_2
\]
Practice — How many formula units are in 50.0 g of PbO₂? (PbO₂ = 239.2)

1 mol PbO₂ = 239.2 g, 1 mol = 6.022 \times 10^{23}

\[
50.0 \text{ g PbO}_2 \times \frac{1 \text{ mol PbO}_2}{239.2 \text{ g PbO}_2} \times \frac{6.022 \times 10^{23} \text{ units}}{1 \text{ mol}} = 1.26 \times 10^{23} \text{ units PbO}_2
\]
Practice — What is the mass of $4.78 \times 10^{24}$ NO$_2$ molecules?

1 mol NO$_2$ = 46.01 g, 1 mol = $6.022 \times 10^{23}$

$4.78 \times 10^{24}$ molec NO$_2$ × $\frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ molec}}$ × $\frac{46.01 \text{ g}}{1 \text{ mol NO}_2}$

= 365 g NO$_2$
Percent Composition
Percent Composition

Percentage of each element in a compound by mass

Can be determined from

1. the formula of the compound
2. the experimental mass analysis of the compound
Find the mass percent of Cl in $C_2Cl_4F_2$

Mass % Cl = $\frac{4 \times \text{molar mass Cl}}{\text{molar mass } C_2Cl_4F_2} \times 100\%$

molar mass $C_2Cl_4F_2 = 2(12.01) + 4(35.45) + 2(19.00) = 203.8 \text{ g/mol}$

$\text{Mass % Cl} = \frac{141.8 \text{ g/mol}}{203.8 \text{ g/mol}} \times 100\% = 69.58\%$
Practice — Determine the mass percent composition of the following $\text{CaCl}_2$

$$\text{Mass} \% \text{ Ca} = \frac{\text{molar mass Ca}}{\text{molar mass CaCl}_2} \times 100\%$$

$$\text{Mass} \% \text{ Cl} = \frac{2 \times \text{molar mass Cl}}{\text{molar mass CaCl}_2} \times 100\%$$

\[2 \times \text{molar mass Cl} = 2(35.45 \text{ g/mol}) = 70.90 \text{ g/mol}\]

\[\text{molar mass CaCl}_2 = 1(40.08) + 2(35.45) = 110.98 \text{ g/mol}\]

$$\text{Mass} \% \text{ Ca} = \frac{40.08 \text{ g/mol}}{110.98 \text{ g/mol}} \times 100\% = 36.11\%$$

$$\text{Mass} \% \text{ Cl} = \frac{70.90 \text{ g/mol}}{110.98 \text{ g/mol}} \times 100\% = 63.88\%$$
Mass Percent as a Conversion Factor

If NaCl is 39% sodium, find the mass of table salt containing 2.4 g of Na.

\[
g_{\text{Na}} \rightarrow g_{\text{NaCl}}
\]

\[
\frac{100 \text{ g NaCl}}{39 \text{ g Na}}
\]

\[
2.4 \text{ g Na} \times \frac{100 \text{ g NaCl}}{39 \text{ g Na}} = 6.2 \text{ g NaCl}
\]
Find the mass of sodium in 6.2 g of NaCl

\[
\text{g NaCl} \xrightarrow{\frac{1\text{ mol}}{58.44\text{ g}}} \text{mol NaCl} \xrightarrow{\frac{1\text{ mol Na}}{1\text{ mol NaCl}}} \text{mol Na} \xrightarrow{22.99\text{ g Na}} \text{g Na}
\]

\[
6.2 \text{ g NaCl} \times \frac{1\text{ mol NaCl}}{58.44\text{ g NaCl}} \times \frac{1\text{ mol Na}}{1\text{ mol NaCl}} \times \frac{22.99\text{ g Na}}{1\text{ mol Na}} = 2.4 \text{ g Na}
\]
Empirical Formulas
Empirical Formula

Simplest, whole-number ratio of the atoms of elements in a compound

Can be determined from elemental analysis
Finding an Empirical Formula from % Composition

1. Convert the percentages to grams
2. Convert grams to moles
3. Write a pseudoformula using moles as subscripts
4. Divide all by smallest number of moles
5. Multiply all mole ratios by number to make all whole numbers
Example:
Find the empirical formula of aspirin with the given mass percent composition

Given: $C = 60.00\%$
      $H = 4.48\%$
      $O = 35.53\%$

Therefore, in 100 g of aspirin there are 60.00 g C, 4.48 g H, and 35.53 g O
Manipulate subscripts to obtain whole-number ratio
Calculate the moles of each element

\[ 60.00 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 4.996 \text{ mol C} \]

\[ 4.48 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 4.44 \text{ mol H} \]

\[ 35.53 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 2.220 \text{ mol O} \]

Write a pseudoformula

\[ \text{C}_{4.996}\text{H}_{4.44}\text{O}_{2.220} \]
Find the mole ratio

\[ \text{C}_{2.25}\text{H}_{2.00}\text{O}_{1.00} \]

Multiply subscripts by factor to give whole number

\[ \times 4 \]

\[ \text{C}_9\text{H}_8\text{O}_4 \]
Practice — Determine the empirical formula of stannous fluoride, which contains 75.7% Sn (118.70 g/mol) and the rest fluorine (19.00 g/mol)

Given: 75.7% Sn, \((100 - 75.3) = 24.3\%\) F
Practice — Determine the empirical formula of stannous fluoride, which contains 75.7% Sn (118.70 g/mol) and the rest fluorine (19.00 g/mol)

<table>
<thead>
<tr>
<th>Element</th>
<th>Ratio in Grams</th>
<th>Molar Mass</th>
<th>Ratio in Moles</th>
<th>Ratio in Moles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sn</td>
<td>75.7g</td>
<td>$\frac{1\text{mol}}{118.7g}$</td>
<td>0.6377</td>
<td>1.000</td>
</tr>
<tr>
<td>F</td>
<td>24.3g</td>
<td>$\frac{1\text{mol}}{19.00g}$</td>
<td>1.279</td>
<td>2.005</td>
</tr>
</tbody>
</table>

\[ \text{SnF}_2 \]
Practice — Determine the empirical formula of magnetite, which contains 72.4% Fe (55.85) and the rest oxygen (16.00)

Given: 72.4% Fe, \( (100 - 72.4) = 27.6\% \) O

**Diagram:**
- \( g \text{ Fe} \rightarrow \text{mol Fe} \)
- \( g \text{ O} \rightarrow \text{mol O} \)
- \( \text{pseudo-formula} \)
- \( \text{whole mole number ratio} \rightarrow \text{ratio} \rightarrow \text{empirical formula} \)
Determine the empirical formula of magnetite, which contains 72.4% Fe (55.85) and the rest oxygen (16.00)

<table>
<thead>
<tr>
<th>Element</th>
<th>Ratio in Grams</th>
<th>Molar Mass</th>
<th>Ratio in Moles</th>
<th>Ratio in Moles</th>
<th>Ratio in Moles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
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<td>1mol/55.85</td>
<td>1.296</td>
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<tr>
<td>O</td>
<td>27.6g</td>
<td>1mol/16.00</td>
<td>1.725</td>
<td>1.33</td>
<td>4</td>
</tr>
</tbody>
</table>

**Fe₃O₄**
Molecular Formulas
Molecular Formulas

The molecular formula is a multiple of the empirical formula.

To determine the molecular formula you need to know the empirical formula and the molar mass of the compound.

\[
\frac{\text{Molar Mass}_{\text{molecular formula}}}{\text{Molar Mass}_{\text{empirical formula}}} = \text{multiplying factor, } n
\]
Find the molecular formula of butanedione if its empirical formula is \( \text{C}_2\text{H}_3\text{O} \) and its molar mass (MM) is 86.03 g/mol.

\[
\text{Molar Mass Emp. Form.} = 2(12.01 \text{ g/mol}) + 3(1.008 \text{ g/mol}) + 1(16.00 \text{ g/mol}) = 43.04 \text{ g/mol}
\]

Molecular Formula = \( \text{C}_2\text{H}_3\text{O} \times 2 = \text{C}_4\text{H}_6\text{O}_2 \)
Practice – Benzopyrene has a molar mass of 252 g and an empirical formula of \(\text{C}_5\text{H}_3\). What is its molecular formula? \((\text{C} = 12.01, \text{H}=1.01)\)

\[
\begin{align*}
\text{C}_5 &= 5(12.01 \text{ g}) = 60.05 \text{ g} \\
\text{H}_3 &= 3(1.01 \text{ g}) = 3.03 \text{ g} \\
\text{C}_5\text{H}_3 &= 63.08 \text{ g}
\end{align*}
\]

Molecular formula = \(\{\text{C}_5\text{H}_3\} \times 4 = \text{C}_{20}\text{H}_{12}\)
Combustion Analysis
Combustion Analysis

(Generally used for organic compounds containing C, H, O)

A known mass of compound is burned in oxygen and the masses of the products formed (CO\textsubscript{2} and H\textsubscript{2}O) are determined.

By knowing the masses of the products and composition of constituent elements in the product, the original amount of constituent elements can be determined.

*It is assumed that all of the carbon in the original sample is converted to carbon dioxide and all of the hydrogen in the sample is converted to water.*
Combustion Analysis

- Oxygen added here
- Compound to be analyzed
- Unused oxygen leaves
- Water absorber
- Carbon dioxide absorber
Combustion of a 0.8233 g sample of a compound containing only carbon, hydrogen, and oxygen produced the following:

\[ \text{CO}_2 = 2.445 \text{ g} \quad \text{(This came from C.)} \]
\[ \text{H}_2\text{O} = 0.6003 \text{ g} \quad \text{(This came from H.)} \]

Determine the empirical formula of the compound.
1 mole CO₂ = 44.01 g CO₂  
1 mole H₂O = 18.02 g H₂O  

1 mole C = 12.01 g C  
1 mole H = 1.008 g H  
1 mole O = 16.00 g O  

1 mole CO₂ = 1 mole C  
1 mole H₂O = 2 mole H  

\[
2.445 \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 0.05556 \text{ mol C}
\]

\[
0.6003 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 0.06662 \text{ mol H}
\]

In the original sample
In the original sample

\[0.05556 \text{ mol C} \times \frac{12.01 \text{ g}}{1 \text{ mol C}} = 0.6673 \text{ g C}\]

\[0.06662 \text{ mol H} \times \frac{1.008 \text{ g}}{1 \text{ mol H}} = 0.06715 \text{ g H}\]

\[0.8233 \text{ g compound} - (0.6673 \text{ g C} + 0.06715 \text{ g H}) = 0.0889 \text{ g O}\]

\[0.0889 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g}} = 0.00556 \text{ mol O}\]
Pseudo formula

\[
\frac{C^{0.05556}H^{0.06662}O^{0.00556}}{0.00556} \div 0.00556
\]

Empirical formula

\[
C_{10}H_{12}O_1
\]
Combustion of 0.844 g of caproic acid produced 0.784 g of $\text{H}_2\text{O}$ and 1.92 g of $\text{CO}_2$. If the molar mass of caproic acid is 116.2 g/mol, what is the molecular formula of caproic acid?

\[
1.92 \text{ g CO}_2 \times \frac{1 \text{ mol CO}_2}{44.01 \text{ g CO}_2} \times \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} = 0.0436 \text{ mol C}
\]

\[
0.784 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} \times \frac{2 \text{ mol H}}{1 \text{ mol H}_2\text{O}} = 0.0870 \text{ mol H}
\]
0.844 g compound - (0.524 g C + 0.0877 g H) = 0.232 g O

\[ 0.232 \text{ g O} \times \frac{1 \text{ mol O}}{16.00 \text{ g}} = 0.0145 \text{ mol O} \]

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>H</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>g</td>
<td>0.524</td>
<td>0.0877</td>
<td>0.232</td>
</tr>
<tr>
<td>moles</td>
<td>0.0436</td>
<td>0.0870</td>
<td>0.0145</td>
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</table>

\[
\frac{C_{0.0436} \cdot H_{0.0870} \cdot O_{0.0145}}{0.0145 \cdot 0.0145 \cdot 0.0145} = C_3H_6O_1
\]
Molecular formula \( = \{C_3H_6O\} \times 2 = C_6H_{12}O_2\)