- chemistry is all about the interaction of electrons available for bonding
- grouping is based on number of electrons in orbital relevant for bonding
- atomic number = total number of electrons

- shaded elements are essential for life on Earth
  most of these are important for atmospheric chemistry
  one of the non-shaded elements is also very important for atmospheric chemistry. which one?
Chemical Bonding

• how are electrons “arranged” in atoms and molecules?
  – quantum (“shell”) numbers
  – molecular orbital (MO) theory

• how do electrons interact to form bonds?
  – type of bond (ionic, covalent, “weak”)
  – energy → thermodynamics (“if”)
  – reactivity → kinetics (“when”)

• how can this knowledge help us?
  – activity/reactivity prediction
  – analytical methods and instrumentation
  – modeling
### Solutions to the Schrödinger Equation

\[ \hat{H} \varphi = E \varphi \]

\[ \varphi = f(n, l, m_l) = N \times R_{nl}(r) \times \Phi(lm_l) \]

<table>
<thead>
<tr>
<th>Quantenzahlen der Orbitale</th>
<th>Bezeichnung der Orbitale</th>
<th>Radialfunktion ( R_{nl}(r) )</th>
<th>Winkelabhängige Funktion ( \Phi_{lm_l}(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0 0</td>
<td>1s</td>
<td>( 2e^{-r} )</td>
<td>( \frac{1}{2\sqrt{2}} )</td>
</tr>
<tr>
<td>2 0 0</td>
<td>2s</td>
<td>( \frac{1}{2\sqrt{2}} (r-2)e^{-r/2} )</td>
<td>( \frac{1}{2\sqrt{3}} )</td>
</tr>
<tr>
<td>2 1 (1(^d))</td>
<td>2p_x</td>
<td>( \frac{1}{2\sqrt{2}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{3}}{2\sqrt{2}} (x/r) )</td>
</tr>
<tr>
<td>2 1 (0)</td>
<td>2p_y</td>
<td>( \frac{1}{2\sqrt{2}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{3}}{2\sqrt{2}} (y/r) )</td>
</tr>
<tr>
<td>2 1 (-1(^d))</td>
<td>2p_z</td>
<td>( \frac{1}{2\sqrt{2}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{3}}{2\sqrt{2}} (z/r) )</td>
</tr>
<tr>
<td>3 0 0</td>
<td>3s</td>
<td>( \frac{2}{81\sqrt{3}} (27 - 18r + 2r^2)e^{-r/2} )</td>
<td>( \frac{1}{2\sqrt{3}} )</td>
</tr>
<tr>
<td>3 1 (1(^d))</td>
<td>3p_x</td>
<td>( -\frac{4}{81\sqrt{2}} (r^2 - 6r)e^{-r/2} )</td>
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<tr>
<td>3 2 (2(^d))</td>
<td>3d_{x^2-y^2}</td>
<td>( \frac{4}{81\sqrt{30}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{15}}{4\sqrt{3}} ) ((x^2 - y^2)/r^2)</td>
</tr>
<tr>
<td>3 2 (1(^d))</td>
<td>3d_{xz}</td>
<td>( \frac{4}{81\sqrt{30}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{30}}{2\sqrt{2}} (xz/r^2) )</td>
</tr>
<tr>
<td>3 2 (0)</td>
<td>3d_{x^2}</td>
<td>( \frac{4}{81\sqrt{30}} r^2e^{-r/2} )</td>
<td>( \frac{\sqrt{5}}{4\sqrt{2}} ) ((3x^2 - y^2)/r^2)</td>
</tr>
<tr>
<td>3 2 (-1(^d))</td>
<td>3d_{yz}</td>
<td>( \frac{4}{81\sqrt{30}} r^2e^{-r/2} )</td>
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Orbitals

• Definition

An orbital is a one-electron probability density representation of a solution to the Schrödinger equation.

• Quantum numbers

There are four quantum numbers that completely describe the state an electron is in:

- Main (or shell) quantum number, \( n \)
- Orbital (momentum) quantum number, \( l \)
- Magnetic quantum number, \( m_l \)
- Spin quantum number, \( s \)
s-orbitals

3-D 90\% probability surface
\sim |\varphi|^2

Radial function

(a) s-Orbital

(b) $R(r)$

Knotenflächen

Knotenfläche
p-orbitals

(a) $p_y$-Orbital

(b) $p_x$-Orbital

$2p$

$3p$

Knotenfläche
d-orbitals
Atomic Orbital energy levels

Main quantum number

Energy (relative)

niedrige Energie

hohe Energie
- chemistry is all about the interaction of electrons available for bonding
- grouping is based on number of electrons in outermost shell
- atomic number = total number of electrons

- shaded elements are essential for life on Earth
  - some of these are important for atmospheric chemistry
  - others are naturally only found in the solid phase or in solute in particulate matter, or are inert
  - a group of heavy metals is found in particles due to human activities (mostly not essential, but often toxic for many life forms on earth)