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- Periodic trends in properties of the elements
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etc.)

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Quantum Chemistry C. David Sherrill  
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means “ from the beginning ” or “ from first principles ” . Ab initio quantum chemistry distinguishes itself from other computational methods in that it is based solely on established laws of nature: quantum mechanics Over the last two decades powerful molecular modelling



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Quantum Mechanics in Chemistry  
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of electrons that can fit in a shell:  $2n^2$ .

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The 3 Quantum Numbers Principal

Quantum Number,  $n$  Azimuthal

Quantum Number,  $l$  Magnetic

Quantum Number,  $m_l$  6. Principal

Quantum Number main energy level

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of an orbital. Indicates the relative size of the orbital an increase in  $n$  also means increase in the energy of the electron in the orbital.  $n = 1, 2, 3, \dots$

Introduction to Quantum Chemistry  
QUANTUM CHEMISTRY Mark S.  
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