

PHY 742 Quantum Mechanics II

12-12:50 PM MWF Olin 103

Plan for Lecture 29

Quantum mechanics of a multi electron atom

Analysis of atomic term splittings

1. Energy of closed shells
2. 1 electron outside a closed shell
3. 2 electrons outside a closed shell

25	Mon: 04/04/2022	Chap. 10 (review)	Multiparticle systems and second quantization	#20	04/06/2022
26	Wed: 04/06/2022	Chap. 10 (review)	Multiparticle systems and second quantization		
27	Fri: 04/08/2022		Multi electron atoms	#21	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	#22	04/18/2022
29	Wed: 04/13/2022		Multi electron atoms		
	Fri: 04/15/2022	<i>No class</i>	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons		
31	Wed: 04/20/2022		BCS model of superconductivity		
32	Fri: 04/22/2022		BCS model of superconductivity		

PERIODIC TABLE																	
Atomic Properties of the Elements																	
Group 1 IA 1 ¹H Hydrogen 1.008 1s 13.5984 2 IIA 4 ⁴Be Beryllium 9.0122 1s²2s² 9.3227 3 IIIB 11 ¹¹Na Sodium 22.990 [Ne]3s 5.1391 4 IVB 12 ¹²Mg Magnesium 24.305 [Ne]3s² 7.6462 5 VB 19 ¹⁹K Potassium 39.098 [Ar]4s 4.3407 6 VIB 20 ²⁰Ca Calcium 40.078 [Ar]4s² 6.1132 7 VIIB 21 ²¹Sc Scandium 44.956 [Ar]3d¹4s² 6.2173 8 VIII 22 ²²Ti Titanium 47.887 [Ar]3d²4s² 6.8281 9 VIII 23 ²³V Vanadium 50.942 [Ar]3d³4s² 6.7665 10 VIII 24 ²⁴Cr Chromium 51.996 [Ar]3d⁵4s¹ 7.4300 11 VIII 25 ²⁵Mn Manganese 54.938 [Ar]3d⁵4s² 7.9025 12 IIB 26 ²⁶Fe Iron 55.845 [Ar]3d⁶4s² 7.8100 13 IIB 27 ²⁷Co Cobalt 58.933 [Ar]3d⁷4s² 7.7264 14 IIB 28 ²⁸Ni Nickel 58.693 [Ar]3d⁸4s² 7.6399 15 IIB 29 ²⁹Cu Copper 63.546 [Ar]3d¹⁰4s¹ 7.7264 16 IIB 30 ³⁰Zn Zinc 65.38 [Ar]3d¹⁰4s² 9.3942 17 VIIA 31 ³¹Ga Gallium 69.723 [Ar]3d¹⁰4s²4p¹ 7.8994 18 VIIA 32 ³²Ge Germanium 72.630 [Ar]3d¹⁰4s²4p² 7.8994 19 VIIA 33 ³³As Arsenic 74.922 [Ar]3d¹⁰4s²4p³ 7.8994 20 VIIA 34 ³⁴Se Selenium 78.971 [Ar]3d¹⁰4s²4p⁴ 7.8994 21 VIIA 35 ³⁵Br Bromine 79.904 [Ar]3d¹⁰4s²4p⁵ 11.8138 22 VIIA 36 ³⁶Kr Krypton 83.798 [Ar]3d¹⁰4s²4p⁶ 13.9996 23 VIIA 37 ³⁷Rb Rubidium 85.468 [Kr]5s 4.1771 24 VIIA 38 ³⁸Sr Strontium 87.62 [Kr]5s² 5.6949 25 VIIA 39 ³⁹Y Yttrium 88.906 [Kr]4d¹5s² 6.2173 26 VIIA 40 ⁴⁰Zr Zirconium 91.224 [Kr]4d²5s² 6.6341 27 VIIA 41 ⁴¹Nb Niobium 92.906 [Kr]4d⁴5s¹ 6.7589 28 VIIA 42 ⁴²Mo Molybdenum 95.95 [Kr]4d⁵5s¹ 7.0924 29 VIIA 43 ⁴³Tc Technetium (97) [Kr]4d⁵5s² 7.1194 30 VIIA 44 ⁴⁴Ru Ruthenium 101.07 [Kr]4d⁷5s¹ 7.3605 31 VIIA 45 ⁴⁵Rh Rhodium 106.42 [Kr]4d⁸5s¹ 7.4589 32 VIIA 46 ⁴⁶Pd Palladium 106.42 [Kr]4d¹⁰5s⁰ 8.3369 33 VIIA 47 ⁴⁷Ag Silver 107.87 [Kr]4d¹⁰5s¹ 7.5762 34 VIIA 48 ⁴⁸Cd Cadmium 112.41 [Kr]4d¹⁰5s² 8.9938 35 VIIA 49 ⁴⁹In Indium 114.82 [Kr]4d¹⁰5s²5p¹ 7.5762 36 VIIA 50 ⁵⁰Sn Tin 118.71 [Kr]4d¹⁰5s²5p² 7.3439 37 VIIA 51 ⁵¹Sb Antimony 121.76 [Kr]4d¹⁰5s²5p³ 8.6084 38 VIIA 52 ⁵²Te Tellurium 127.60 [Kr]4d¹⁰5s²5p⁴ 9.0097 39 VIIA 53 ⁵³I Iodine 126.90 [Kr]4d¹⁰5s²5p⁵ 10.4513 40 VIIA 54 ⁵⁴Xe Xenon 131.29 [Kr]4d¹⁰5s²5p⁶ 12.1298 41 VIIA 55 ⁵⁵Cs Cesium 132.91 [Xe]6s 3.8939 42 VIIA 56 ⁵⁶Ba Barium 137.33 [Xe]6s² 5.2117 43 VIIA 57 ⁵⁷La Lanthanum 138.91 [Xe]5d¹6s² 5.5769 44 VIIA 58 ⁵⁸Ce Cerium 140.12 [Xe]4f¹5d¹6s² 5.5386 45 VIIA 59 ⁵⁹Pr Praseodymium 140.91 [Xe]4f³6s² 5.4702 46 VIIA 60 ⁶⁰Nd Neodymium 144.24 [Xe]4f⁴6s² 5.5250 47 VIIA 61 ⁶¹Pm Promethium (145) [Xe]4f⁵6s² 5.577 48 VIIA 62 ⁶²Sm Samarium 150.36 [Xe]4f⁶6s² 5.6437 49 VIIA 63 ⁶³Eu Europium 151.96 [Xe]4f⁷6s² 5.7074 50 VIIA 64 ⁶⁴Gd Gadolinium 157.25 [Xe]4f⁷5d¹6s² 6.1498 51 VIIA 65 ⁶⁵Tb Terbium 158.93 [Xe]4f⁹6s² 5.8638 52 VIIA 66 ⁶⁶Dy Dysprosium 162.50 [Xe]4f¹⁰6s² 5.9391 53 VIIA 67 ⁶⁷Ho Holmium 164.93 [Xe]4f¹¹6s² 6.0215 54 VIIA 68 ⁶⁸Er Erbium 167.26 [Xe]4f¹²6s² 6.1077 55 VIIA 69 ⁶⁹Tm Thulium 168.93 [Xe]4f¹³6s² 6.1843 56 VIIA 70 ⁷⁰Yb Ytterbium 173.05 [Xe]4f¹⁴6s² 6.2542 57 VIIA 71 ⁷¹Lu Lutetium 174.97 [Xe]4f¹⁴5d¹6s² 6.4259 58 VIIA 89 ⁸⁹Ac Actinium (227) [Rn]6s²5f⁷7s² 5.3802 59 VIIA 90 ⁹⁰Th Thorium 232.04 [Rn]6s²5f¹⁴7s² 6.3067 60 VIIA 91 ⁹¹Pa Protactinium 231.04 [Rn]5f²6s²7s² 5.89 61 VIIA 92 ⁹²U Uranium 238.03 [Rn]5f³6s²7s² 6.1941 62 VIIA 93 ⁹³Np Neptunium (237) [Rn]5f⁴6s²7s² 6.2655 63 VIIA 94 ⁹⁴Pu Plutonium (244) [Rn]5f⁶6s²7s² 6.0288 64 VIIA 95 ⁹⁵Am Americium (243) [Rn]5f⁷6s²7s² 5.9738 65 VIIA 96 ⁹⁶Cm Curium (247) [Rn]5f⁸6s²7s² 5.9914 66 VIIA 97 ⁹⁷Bk Berkelium (247) [Rn]5f⁹6s²7s² 6.1978 67 VIIA 98 ⁹⁸Cf Californium (251) [Rn]5f¹⁰6s²7s² 6.2817 68 VIIA 99 ⁹⁹Es Einsteinium (252) [Rn]5f¹¹6s²7s² 6.3676 69 VIIA 100 ¹⁰⁰Fm Fermium (257) [Rn]5f¹²6s²7s² 6.50 70 VIIA 101 ¹⁰¹Md Mendelevium (258) [Rn]5f¹³6s²7s² 6.58 71 VIIA 102 ¹⁰²No Nobelium (259) [Rn]5f¹⁴6s²7s² 6.66 72 VIIA 103 ¹⁰³Lr Lawrencium (260) [Rn]5f¹⁴6s²7p¹ 4.96 Atomic Number Ground State Symbol Name Standard Atomic Weight (u) Ground-state Configuration Ionization Energy (eV) 58 ⁵⁸Ce Cerium 140.12 [Xe]4f¹5d¹6s² 5.5386 13 IIIA 5 ⁵B Boron 10.81 1s²2s²2p¹ 8.2990 14 IVA 6 ⁶C Carbon 12.011 1s²2s²2p² 11.2603 15 VA 7 ⁷N Nitrogen 14.007 1s²2s²2p³ 14.5341 16 VIA 8 ⁸O Oxygen 15.999 1s²2s²2p⁴ 13.6181 17 VIIA 9 ⁹F Fluorine 18.998 1s²2s²2p⁵ 17.4228 18 VIIA 10 ¹⁰Ne Neon 20.180 1s²2s²2p⁶ 21.5645 13 IIIA 13 ¹³Al Aluminum 26.982 [Ne]3s²3p¹ 5.9859 14 IVA 14 ¹⁴Si Silicon 28.086 [Ne]3s²3p² 8.1517 15 VA 15 ¹⁵P Phosphorus 30.974 [Ne]3s²3p³ 10.4867 16 VIA 16 ¹⁶S Sulfur 32.06 [Ne]3s²3p⁴ 10.3600 17 VIIA 17 ¹⁷Cl Chlorine 35.45 [Ne]3s²3p⁵ 12.9676 18 VIIA 18 ¹⁸Ar Argon 39.948 [Ne]3s²3p⁶ 15.7596 13 IIIA 31 ³¹Ga Gallium 69.723 [Ar]3d¹⁰4s²4p¹ 7.8994 14 IVA 32 ³²Ge Germanium 72.630 [Ar]3d¹⁰4s²4p² 7.8994 15 VA 33 ³³As Arsenic 74.922 [Ar]3d¹⁰4s²4p³ 7.8996 16 VIA 34 ³⁴Se Selenium 78.971 [Ar]3d¹⁰4s²4p⁴ 7.824 17 VIIA 35 ³⁵Br Bromine 79.904 [Ar]3d¹⁰4s²4p⁵ 11.8138 18 VIIA 36 ³⁶Kr Krypton 83.798 [Ar]3d¹⁰4s²4p⁶ 13.9996 13 IIIA 49 ⁴⁹In Indium 114.82 [Kr]4d¹⁰5s²5p¹ 7.5762 14 IVA 50 ⁵⁰Sn Tin 118.71 [Kr]4d¹⁰5s²5p² 7.3439 15 VA 51 ⁵¹Sb Antimony 121.76 [Kr]4d¹⁰5s²5p³ 8.6084 16 VIA 52 ⁵²Te Tellurium 127.60 [Kr]4d¹⁰5s²5p⁴ 9.0097 17 VIIA 53 ⁵³I Iodine 126.90 [Kr]4d¹⁰5s²5p⁵ 10.4513 18 VIIA 54 ⁵⁴Xe Xenon 131.29 [Kr]4d¹⁰5s²5p⁶ 12.1298 13 IIIA 81 ⁸¹Tl Thallium 204.38 [Xe]4f¹⁴5d¹⁰6s²6p¹ 6.1033 14 IVA 82 ⁸²Pb Lead 207.2 [Xe]4f¹⁴5d¹⁰6s²6p² 7.4167 15 VA 83 ⁸³Bi Bismuth 208.98 [Xe]4f¹⁴5d¹⁰6s²6p³ 7.2855 16 VIA 84 ⁸⁴Po Polonium (209) [Xe]4f¹⁴5d¹⁰6s²6p⁴ 8.414 17 VIIA 85 ⁸⁵At Astatine (210) [Xe]4f¹⁴5d¹⁰6s²6p⁵ 9.3175 18 VIIA 86 ⁸⁶Rn Radon (222) [Xe]4f¹⁴5d¹⁰6s²6p⁶ 10.7485 13 IIIA 113 ¹¹³Nh Nihonium (286) [Xe]4f¹⁴5d¹⁰6s²6p¹ 6.1978 14 IVA 114 ¹¹⁴Fl Flerovium (289) [Xe]4f¹⁴5d¹⁰6s²6p² 6.3676 15 VA 115 ¹¹⁵Mc Moscovium (289) [Xe]4f¹⁴5d¹⁰6s²6p³ 6.50 16 VIA 116 ¹¹⁶Lv Livermorium (293) [Xe]4f¹⁴5d¹⁰6s²6p⁴ 6.58 17 VIIA 117 ¹¹⁷Ts Tennessine (294) [Xe]4f¹⁴5d¹⁰6s²6p⁵ 6.66 18 VIIA 118 ¹¹⁸Og Oganesson (294) [Xe]4f¹⁴5d¹⁰6s²6p⁶ 4.96 13 IIIA 5 ⁵B Boron 10.81 1s²2s²2p¹ 8.2990 14 IVA 6 ⁶C Carbon 12.011 1s²2s²2p² 11.2603 15 VA 7 ⁷N Nitrogen 14.007 1s²2s²2p³ 14.5341 16 VIA 8 ⁸O Oxygen 15.999 1s²2s²2p⁴ 13.6181 17 VIIA 9 ⁹F Fluorine 18.998 1s²2s²2p⁵ 17.4228 18 VIIA 10 ¹⁰Ne Neon 20.180 1s²2s²2p⁶ 21.5645 13 IIIA 13 ¹³Al Aluminum 26.982 [Ne]3s²3p¹ 5.9859 14 IVA 14 ¹⁴Si 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Closed shell

2

¹S₀

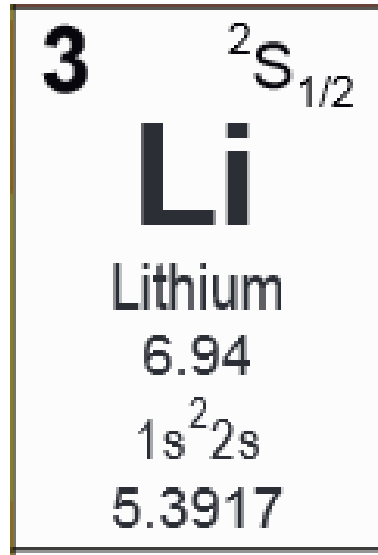
He

Helium

4.0026

1s²

24.5874



PERIODIC TABLE

Atomic Properties of the Elements

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANT¹

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ^{133}Cs

speed of light in vacuum c 299 792 458 m s^{-1} (exact)

Planck constant h 6.626 070 15 $\times 10^{-34}$ J Hz^{-1} (exact)

elementary charge e 1.602 176 634 $\times 10^{-19}$ C (exact)

Avogadro constant N_A 6.022 140 76 $\times 10^{23}$ mol^{-1} (exact)

Boltzmann constant k 1.380 649 $\times 10^{-23}$ J K^{-1} (exact)

electron volt eV 1.602 176 634 $\times 10^{-19}$ J (exact)

electron mass m_e 9.109 383 70 $\times 10^{-31}$ kg (exact)

energy equivalent $m_e c^2$ 0.510 998 950 MeV (exact)

proton mass m_p 1.672 621 924 $\times 10^{-27}$ kg (exact)

energy equivalent $m_p c^2$ 938.272 088 MeV (exact)

fine-structure constant α 1/137.035 999 (exact)

Rydberg energy $R_\infty h c$ 13.605 693 1230 eV (exact)

Newtonian constant of gravitation G 6.674 $\times 10^{-11}$ $\text{m}^3 \text{kg}^{-1} \text{s}^{-2}$

¹For the most accurate values of these and other constants, visit pml.nist.gov/constants.

Physical Measurement Laboratory www.nist.gov/pml

Standard Reference Data www.nist.gov/srd

NIST National Institute of Standards and Technology U.S. Department of Commerce

18 VIIIA

2 He $1s^2$

13 IIIA 14 IVA 15 VA 16 VIA 17 VIIA

5 B $2s^2 2p^1$ 6 C $2s^2 2p^2$ 7 N $2s^2 2p^3$ 8 O $2s^2 2p^4$ 9 F $2s^2 2p^5$ 10 Ne $2s^2 2p^6$

Boron 10.81 $1s^2 2s^2 2p^1$ Carbon 12.011 $1s^2 2s^2 2p^2$ Nitrogen 14.007 $1s^2 2s^2 2p^3$ Oxygen 15.999 $1s^2 2s^2 2p^4$ Fluorine 18.998 $1s^2 2s^2 2p^5$ Neon 20.180 $1s^2 2s^2 2p^6$

11 IB 12 IIB

3 4 5 6 7 8 9 10 11 12

IIIA IVB VB VIB VIIB VIIIB VIII IB IIB

19 K $3s^2 3p^6 4s^1$ 20 Ca $3s^2 3p^6 4s^2$ 21 Sc $3d^1 4s^2$ 22 Ti $3d^2 4s^2$ 23 V $3d^3 4s^2$ 24 Cr $3d^5 4s^1$ 25 Mn $3d^5 4s^2$ 26 Fe $3d^6 4s^2$ 27 Co $3d^7 4s^2$ 28 Ni $3d^8 4s^2$ 29 Cu $3d^9 4s^1$ 30 Zn $3d^{10} 4s^2$

Potassium 39.098 $[\text{Ar}]4s^1$ Calcium 40.078 $[\text{Ar}]4s^2$ Scandium 44.956 $[\text{Ar}]3d^1 4s^2$ Titanium 47.867 $[\text{Ar}]3d^2 4s^2$ Vanadium 50.942 $[\text{Ar}]3d^3 4s^2$ Chromium 51.996 $[\text{Ar}]3d^5 4s^1$ Manganese 54.938 $[\text{Ar}]3d^5 4s^2$ Iron 55.845 $[\text{Ar}]3d^6 4s^2$ Cobalt 58.933 $[\text{Ar}]3d^7 4s^2$ Nickel 58.693 $[\text{Ar}]3d^8 4s^2$ Copper 63.546 $[\text{Ar}]3d^9 4s^1$ Zinc 65.38 $[\text{Ar}]3d^{10} 4s^2$

37 Rb $4s^2 4p^6 5s^1$ 38 Sr $4s^2 4p^6 5s^2$ 39 Y $4d^1 5s^2$ 40 Zr $4d^2 5s^2$ 41 Nb $4d^4 5s^1$ 42 Mo $4d^5 5s^1$ 43 Tc $4d^5 5s^2$ 44 Ru $4d^7 5s^1$ 45 Rh $4d^8 5s^1$ 46 Pd $4d^9 5s^1$ 47 Ag $4d^9 5s^1$ 48 Cd $4d^{10} 5s^2$

Rubidium 85.468 $[\text{Kr}]5s^1$ Strontium 87.62 $[\text{Kr}]5s^2$ Yttrium 88.906 $[\text{Kr}]4d^1 5s^2$ Zirconium 91.224 $[\text{Kr}]4d^2 5s^2$ Niobium 92.906 $[\text{Kr}]4d^4 5s^1$ Molybdenum 95.95 $[\text{Kr}]4d^5 5s^1$ Technetium (97) $[\text{Kr}]4d^5 5s^2$ Ruthenium 101.07 $[\text{Kr}]4d^7 5s^1$ Rhodium 106.42 $[\text{Kr}]4d^8 5s^1$ Palladium 106.42 $[\text{Kr}]4d^9 5s^1$ Silver 107.87 $[\text{Kr}]4d^9 5s^1$ Cadmium 112.41 $[\text{Kr}]4d^{10} 5s^2$

55 Cs $5s^2 5p^6 6s^1$ 56 Ba $5s^2 5p^6 6s^2$ 57 La $5d^1 6s^2$ 58 Ce $5d^1 6s^2$ 59 Pr $5d^1 6s^2$ 60 Nd $5d^1 6s^2$ 61 Pm $5d^4 6s^2$ 62 Sm $5d^1 6s^2$ 63 Eu $5d^0 6s^2$ 64 Gd $5d^1 6s^2$ 65 Tb $5d^4 6s^2$ 66 Dy $5d^4 6s^2$ 67 Ho $5d^4 6s^2$ 68 Er $5d^4 6s^2$ 69 Tm $5d^4 6s^2$ 70 Yb $5d^4 6s^2$ 71 Lu $5d^1 6s^2$

Cesium 132.91 $[\text{Xe}]6s^1$ Barium 137.33 $[\text{Xe}]6s^2$ Lanthanum 138.91 $[\text{Xe}]5d^1 6s^2$ Cerium 140.12 $[\text{Xe}]4f^1 5d^1 6s^2$ Praseodymium 140.91 $[\text{Xe}]4f^3 6s^2$ Neodymium 144.24 $[\text{Xe}]4f^4 6s^2$ Promethium (145) $[\text{Xe}]4f^5 6s^2$ Samarium 150.36 $[\text{Xe}]4f^6 6s^2$ Europium 151.96 $[\text{Xe}]4f^7 6s^2$ Gadolinium 157.25 $[\text{Xe}]4f^7 5d^1 6s^2$ Terbium 158.93 $[\text{Xe}]4f^9 6s^2$ Dysprosium 162.50 $[\text{Xe}]4f^10 6s^2$ Holmium 164.93 $[\text{Xe}]4f^{11} 6s^2$ Erbium 167.26 $[\text{Xe}]4f^{12} 6s^2$ Thulium 168.93 $[\text{Xe}]4f^{13} 6s^2$ Ytterbium 173.05 $[\text{Xe}]4f^{14} 6s^2$ Lutetium 174.97 $[\text{Xe}]4f^{14} 5d^1 6s^2$

87 Fr $5s^2 5p^6 6s^2 6p^6 7s^1$ 88 Ra $5s^2 5p^6 6s^2 6p^6 7s^2$ 89 Ac $6d^1 7s^2$ 90 Th $6d^2 7s^2$ 91 Pa $5f^2 6d^1 7s^2$ 92 U $5f^3 6d^1 7s^2$ 93 Np $5f^4 6d^1 7s^2$ 94 Pu $5f^6 6d^1 7s^2$ 95 Am $5f^7 7s^2$ 96 Cm $5f^7 6d^1 7s^2$ 97 Bk $5f^7 6d^1 7s^2$ 98 Cf $5f^10 7s^2$ 99 Es $5f^{11} 7s^2$ 100 Fm $5f^{12} 7s^2$ 101 Md $5f^{13} 7s^2$ 102 No $5f^{14} 7s^2$ 103 Lr $5f^{14} 6d^1 7s^2$

Francium (223) $[\text{Rn}]7s^1$ Radium (226) $[\text{Rn}]7s^2$ Actinium (227) $[\text{Rn}]5f^1 6d^1 7s^2$ Thorium (232) $[\text{Rn}]6d^2 7s^2$ Protactinium (231) $[\text{Rn}]5f^2 6d^1 7s^2$ Uranium (238) $[\text{Rn}]5f^3 6d^1 7s^2$ Neptunium (237) $[\text{Rn}]5f^4 6d^1 7s^2$ Plutonium (244) $[\text{Rn}]5f^6 6d^1 7s^2$ Americium (243) $[\text{Rn}]5f^7 7s^2$ Curium (247) $[\text{Rn}]5f^7 6d^1 7s^2$ Berkelium (247) $[\text{Rn}]5f^7 6d^1 7s^2$ Californium (251) $[\text{Rn}]5f^{10} 7s^2$ Einsteinium (252) $[\text{Rn}]5f^{11} 7s^2$ Fermium (257) $[\text{Rn}]5f^{12} 7s^2$ Mendelevium (258) $[\text{Rn}]5f^{13} 7s^2$ Nobelium (259) $[\text{Rn}]5f^{14} 7s^2$ Lawrencium (260) $[\text{Rn}]5f^{14} 6d^1 7s^2$

104 Rf $5f^{14} 6d^2 7s^2$ 105 Db $5f^{14} 6d^3 7s^2$ 106 Sg $5f^{14} 6d^4 7s^2$ 107 Bh $5f^{14} 6d^5 7s^2$ 108 Hs $5f^{14} 6d^6 7s^2$ 109 Mt $5f^{14} 6d^7 7s^2$ 110 Ds $5f^{14} 6d^8 7s^2$ 111 Rg $5f^{14} 6d^9 7s^2$ 112 Cn $5f^{14} 6d^{10} 7s^2$ 113 Nh $5f^{14} 6d^{10} 7s^2$ 114 Fl $5f^{14} 6d^{10} 7s^2$ 115 Mc $5f^{14} 6d^{10} 7s^2$ 116 Lv $5f^{14} 6d^{10} 7s^2$ 117 Ts $5f^{14} 6d^{10} 7s^2$ 118 Og $5f^{14} 6d^{10} 7s^2$

Rutherfordium (261) $[\text{Rn}]5f^{14} 6d^2 7s^2$ Dubnium (268) $[\text{Rn}]5f^{14} 6d^3 7s^2$ Seaborgium (266) $[\text{Rn}]5f^{14} 6d^4 7s^2$ Bohrium (264) $[\text{Rn}]5f^{14} 6d^5 7s^2$ Hassium (265) $[\text{Rn}]5f^{14} 6d^6 7s^2$ Meitnerium (276) $[\text{Rn}]5f^{14} 6d^7 7s^2$ Darmstadtium (281) $[\text{Rn}]5f^{14} 6d^8 7s^2$ Roentgenium (282) $[\text{Rn}]5f^{14} 6d^9 7s^2$ Copernicium (285) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Nihonium (286) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Flerovium (289) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Moscovium (289) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Livermorium (293) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Tennessine (294) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$ Oganesson (294) $[\text{Rn}]5f^{14} 6d^{10} 7s^2$

Atomic Number Ground State

Symbol

Name

Standard Atomic Weight (u)

Ground-state Configuration Ionization Energy (eV)

58 Ce $1s^2 2s^2 2p^6 3s^2 3p^6 3d^10 4s^2 4p^6 4d^10 5s^2 5p^6 5d^1 6s^2$

Cerium 140.12 $[\text{Xe}]4f^1 5d^1 6s^2$ 5.5386

¹Based upon ^{12}C . () Indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciaaw.org and pml.nist.gov/data. NIST SP 966 (July 2019)

One electron outside a closed shell

PERIODIC TABLE

Atomic Properties of the Elements

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS¹

¹second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s ⁻¹	(exact)
Planck constant	<i>h</i>	6.626 070 15 × 10 ⁻³⁴ J Hz ⁻¹	(exact)
elementary charge	<i>e</i>	1.602 176 634 × 10 ⁻¹⁹ C	(exact)
Avogadro constant	<i>N_A</i>	6.022 140 76 × 10 ²³ mol ⁻¹	(exact)
Boltzmann constant	<i>k</i>	1.380 649 × 10 ⁻²³ J K ⁻¹	(exact)
electron volt	eV	1.602 176 634 × 10 ⁻¹⁹ J	(exact)
electron mass	<i>m_e</i>	9.109 383 70 × 10 ⁻³¹ kg	(exact)
energy equivalent	<i>m_ec²</i>	0.510 998 950 MeV	(exact)
proton mass	<i>m_p</i>	1.672 621 924 × 10 ⁻²⁷ kg	(exact)
energy equivalent	<i>m_pc²</i>	938.272 088 MeV	(exact)
fine-structure constant	<i>α</i>	1/137.035 999	(exact)
Rydberg energy	<i>R_∞hc</i>	13.605 693 1230 eV	(exact)
Newtonian constant of gravitation	<i>G</i>	6.674 × 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻²	(exact)

¹For the most accurate values of these and other constants, visit physics.nist.gov/constants.

- Solids
- Liquids
- Gases
- Artificially Prepared

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
IA	IIA	IIIB	IVB	VB	VIB	VII	VIII	IX	X	XI	XII	IIIB	IVA	VA	VIA	VIIA	VIIIA	
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
H Hydrogen 1.008 1s	He Helium 4.0026 1s	Li Lithium 6.94 1s ² 2s	Be Beryllium 9.0122 1s ² 2s ²	B Boron 10.81 1s ² 2s ² 2p	C Carbon 12.011 1s ² 2s ² 2p ²	N Nitrogen 14.007 1s ² 2s ² 2p ³	O Oxygen 15.999 1s ² 2s ² 2p ⁴	F Fluorine 18.998 1s ² 2s ² 2p ⁵	Ne Neon 20.180 1s ² 2s ² 2p ⁶	Na Sodium 22.990 [Ne]3s	Mg Magnesium 24.305 [Ne]3s ²	Al Aluminum 26.982 [Ne]3s ² 3p	Si Silicon 28.085 [Ne]3s ² 3p ²	P Phosphorus 30.974 [Ne]3s ² 3p ³	S Sulfur 32.06 [Ne]3s ² 3p ⁴	Cl Chlorine 35.45 [Ne]3s ² 3p ⁵	Ar Argon 39.948 [Ne]3s ² 3p ⁶	
K Potassium 39.098 [Ar]4s	Ca Calcium 40.078 [Ar]4s	Sc Scandium 44.956 [Ar]3d ¹ 4s	Ti Titanium 47.867 [Ar]3d ² 4s	V Vanadium 50.942 [Ar]3d ³ 4s	Cr Chromium 51.996 [Ar]3d ⁵ 4s	Mn Manganese 54.938 [Ar]3d ⁵ 4s	Fe Iron 55.845 [Ar]3d ⁶ 4s	Co Cobalt 58.933 [Ar]3d ⁷ 4s	Ni Nickel 58.693 [Ar]3d ⁸ 4s	Cu Copper 63.546 [Ar]3d ¹⁰ 4s	Zn Zinc 65.38 [Ar]3d ¹⁰ 4s	Ga Gallium 69.723 [Ar]3d ¹⁰ 4s ² 4p	Ge Germanium 72.630 [Ar]3d ¹⁰ 4s ² 4p ²	As Arsenic 74.922 [Ar]3d ¹⁰ 4s ² 4p ³	Se Selenium 78.971 [Ar]3d ¹⁰ 4s ² 4p ⁴	Br Bromine 79.904 [Ar]3d ¹⁰ 4s ² 4p ⁵	Kr Krypton 83.798 [Ar]3d ¹⁰ 4s ² 4p ⁶	
Rb Rubidium 85.468 [Kr]5s	Sr Strontium 87.62 [Kr]5s	Y Yttrium 88.906 [Kr]4d ¹ 5s	Zr Zirconium 91.224 [Kr]4d ² 5s	Nb Niobium 92.906 [Kr]4d ⁴ 5s	Mo Molybdenum 95.94 [Kr]4d ⁵ 5s	Tc Technetium (97) [Kr]4d ⁵ 5s	Ru Ruthenium 101.07 [Kr]4d ⁷ 5s	Rh Rhodium 102.91 [Kr]4d ⁸ 5s	Pd Palladium 106.42 [Kr]4d ¹⁰ 5s	Ag Silver 107.87 [Kr]4d ¹⁰ 5s	Cd Cadmium 112.41 [Kr]4d ¹⁰ 5s	In Indium 114.82 [Kr]4d ¹⁰ 5s ² 5p	Sn Tin 118.71 [Kr]4d ¹⁰ 5s ² 5p ²	Sb Antimony 121.76 [Kr]4d ¹⁰ 5s ² 5p ³	Te Tellurium 127.60 [Kr]4d ¹⁰ 5s ² 5p ⁴	I Iodine 126.90 [Kr]4d ¹⁰ 5s ² 5p ⁵	Xe Xenon 131.29 [Kr]4d ¹⁰ 5s ² 5p ⁶	
Cs Cesium 132.91 [Xe]6s	Ba Barium 137.33 [Xe]6s	Hf Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s	Ta Tantalum 180.95 [Xe]4f ¹⁴ 5d ³ 6s	W Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s	Re Rhenium 186.21 [Xe]4f ¹⁴ 5d ⁵ 6s	Os Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s	Ir Iridium 192.22 [Xe]4f ¹⁴ 5d ⁷ 6s	Pt Platinum 195.08 [Xe]4f ¹⁴ 5d ⁹ 6s	Au Gold 196.97 [Xe]4f ¹⁴ 5d ¹⁰ 6s	Hg Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s	Tl Thallium 204.38 [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	Pb Lead 207.2 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ²	Bi Bismuth 208.98 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ³	Po Polonium (209) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁴	At Astatine (210) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁵	Rn Radon (222) [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁶		
Fr Francium (223) [Rn]7s	Ra Radium (226) [Rn]7s	Rf Rutherfordium (261) [Rn]5f ¹⁴ 6d ² 7s	Db Dubnium (268) [Rn]5f ¹⁴ 6d ³ 7s	Sg Seaborgium (266) [Rn]5f ¹⁴ 6d ⁴ 7s	Bh Bohrium (264) [Rn]5f ¹⁴ 6d ⁵ 7s	Hs Hassium (277) [Rn]5f ¹⁴ 6d ⁶ 7s	Mt Meitnerium (268) [Rn]5f ¹⁴ 6d ⁷ 7s	Ds Darmstadtium (271) [Rn]5f ¹⁴ 6d ⁸ 7s	Rg Roentgenium (282) [Rn]5f ¹⁴ 6d ⁹ 7s	Cn Copernicium (285) [Rn]5f ¹⁴ 6d ¹⁰ 7s	Nh Nihonium (286) [Rn]5f ¹⁴ 6d ¹⁰ 7s ¹	Fl Flerovium (289) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²	Mc Moscovium (288) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ³	Lv Livermorium (293) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴	Ts Tennessine (294) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁵	Og Oganesson (294) [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶		

Atomic Number	Ground State
58 ² G ₄	
Ce Cerium 140.12 [Xe]4f ¹ 5d ¹ 6s ²	
Ac Actinium (227) [Rn]5f ¹ 7s	
Th Thorium 232.04 [Rn]5f ² 7s	
Pa Protactinium 231.04 [Rn]5f ² 6d ¹ 7s	
U Uranium 238.03 [Rn]5f ³ 7s	
Np Neptunium (237) [Rn]5f ⁴ 7s	
Pu Plutonium (244) [Rn]5f ⁶ 7s	
Am Americium (243) [Rn]5f ⁷ 7s	
Cm Curium (247) [Rn]5f ⁸ 7s	
Bk Berkelium (247) [Rn]5f ⁹ 7s	
Cf Californium (251) [Rn]5f ¹⁰ 7s	
Es Einsteinium (252) [Rn]5f ¹¹ 7s	
Fm Fermium (257) [Rn]5f ¹² 7s	
Md Mendelevium (258) [Rn]5f ¹³ 7s	
No Nobelium (259) [Rn]5f ¹⁴ 7s	
Lr Lawrencium (260) [Rn]5f ¹⁴ 7s ¹	

¹Based upon ¹²C. () Indicates the mass number of the longest-lived isotope.

For the most precise values and uncertainties visit ciaaw.org and physics.nist.gov/data.

NIST SP 966 (July 2019)

2 electrons outside a closed shell

2 electrons outside a closed shell

Group
1
IA

1
¹H
Hydrogen
1.008
1s
13.5984

2
IIA

4
⁹Be
Beryllium
9.0122
1s²2s²
9.3227

11
IIIB

12
¹¹Na
Sodium
22.990
[Ne]3s
5.1391

19
IVB

20
¹⁹K
Potassium
39.098
[Ar]4s
4.3407

27
VB

28
³⁷Rb
Rubidium
85.468
[Kr]5s
4.1771

35
VIB

36
⁵⁵Cs
Cesium
132.91
[Xe]6s
3.8939

43
VIIB

44
⁸⁷Fr
Francium
(223)
[Rn]7s
4.0727

51
VIIIB

52
⁵⁶Ba
Barium
137.33
[Xe]6s²
5.2117

59
IIIB

60
⁸⁸Ra
Radium
(226)
[Rn]7s²
5.2784

67
IVB

68
¹³⁸La
Lanthanum
138.91
[Xe]5d¹6s²

75
VB

76
¹⁴⁰Ce
Cerium
140.12
[Xe]4f¹5d¹6s²
5.5386

83
VIB

84
¹⁴⁰Pr
Praseodymium
140.91
[Xe]4f³6s²
5.4702

91
VIIB

92
¹⁴⁴Nd
Neodymium
144.24
[Xe]4f⁴6s²
5.5280

99
IIB

100
¹⁴⁵Pm
Promethium
(145)
[Xe]4f⁵6s²
5.577

107
IIIB

108
¹⁵⁰Sm
Samarium
150.36
[Xe]4f⁶6s²
5.6437

115
IVB

116
¹⁵¹Eu
Europium
151.96
[Xe]4f⁷6s²
5.6704

123
VB

124
¹⁵⁷Gd
Gadolinium
157.25
[Xe]4f⁷5d¹6s²
6.1498

131
VIB

132
¹⁵⁸Tb
Terbium
158.93
[Xe]4f⁹6s²
5.8638

139
VIIB

140
¹⁶²Dy
Dysprosium
162.50
[Xe]4f¹⁰6s²
5.9391

147
IIB

148
¹⁶⁴Ho
Holmium
164.93
[Xe]4f¹¹6s²
6.0215

155
IIIB

156
¹⁶⁷Er
Erbium
167.26
[Xe]4f¹²6s²
6.1077

163
IVB

164
¹⁶⁸Tm
Thulium
168.93
[Xe]4f¹³6s²
6.1843

171
VB

172
¹⁷³Yb
Ytterbium
173.05
[Xe]4f¹⁴6s²
6.2542

179
VIB

180
¹⁷⁵Lu
Lutetium
174.97
[Xe]4f¹⁴5d¹6s²
5.4259

187
VIIB

188
²²⁷Ac
Actinium
(227)
[Rn]6d¹7s²
5.3802

195
IIB

196
²³²Th
Thorium
232.04
[Rn]6d²7s²
6.3067

203
IIIB

204
²³¹Pa
Protactinium
231.04
[Rn]5f²6d¹7s²
5.89

211
IVB

212
²³⁸U
Uranium
238.03
[Rn]5f³6d¹7s²
6.1941

219
VB

220
²³⁷Np
Neptunium
(237)
[Rn]5f⁴6d¹7s²
6.2695

227
VIB

228
²⁴⁴Pu
Plutonium
(244)
[Rn]5f⁶7s²
6.0258

235
VIIB

236
²⁴³Am
Americium
(243)
[Rn]5f⁷7s²
5.9738

243
IIB

244
²⁴⁷Cm
Curium
(247)
[Rn]5f⁸7s²
5.9914

251
IIIB

252
²⁴⁷Bk
Berkelium
(247)
[Rn]5f⁹7s²
6.1978

259
IVB

260
²⁵¹Cf
Californium
(251)
[Rn]5f¹⁰7s²
6.2817

267
VB

268
²⁵²Es
Einsteinium
(252)
[Rn]5f¹¹7s²
6.3676

275
VIB

276
²⁵⁷Fm
Fermium
(257)
[Rn]5f¹²7s²
6.80

283
VIIB

284
²⁵⁸Md
Mendelevium
(258)
[Rn]5f¹³7s²
6.58

291
IIB

292
²⁵⁹No
Nobelium
(259)
[Rn]5f¹⁴7s²
6.66

299
IIIB

300
²⁶⁰Lr
Lawrencium
(260)
[Rn]5f¹⁴7s²7p¹
4.96

307
IVB

308
²⁶¹La
Lanthanum
138.91
[Xe]5d¹6s²

315
VB

316
¹⁴⁰Ce
Cerium
140.12
[Xe]4f¹5d¹6s²
5.5386

323
VIB

324
¹⁴⁰Pr
Praseodymium
140.91
[Xe]4f³6s²
5.4702

331
VIIB

332
¹⁴⁴Nd
Neodymium
144.24
[Xe]4f⁴6s²
5.5280

339
IIB

340
¹⁴⁵Pm
Promethium
(145)
[Xe]4f⁵6s²
5.577

347
IIIB

348
¹⁵⁰Sm
Samarium
150.36
[Xe]4f⁶6s²
5.6437

355
IVB

356
¹⁵¹Eu
Europium
151.96
[Xe]4f⁷6s²
5.6704

363
VB

364
¹⁵⁷Gd
Gadolinium
157.25
[Xe]4f⁷5d¹6s²
6.1498

371
VIB

372
¹⁵⁸Tb
Terbium
158.93
[Xe]4f⁹6s²
5.8638

379
VIIB

380
¹⁶²Dy
Dysprosium
162.50
[Xe]4f¹⁰6s²
5.9391

387
IIB

388
¹⁶⁴Ho
Holmium
164.93
[Xe]4f¹¹6s²
6.0215

395
IIIB

396
¹⁶⁷Er
Erbium
167.26
[Xe]4f¹²6s²
6.1077

403
IVB

404
¹⁶⁸Tm
Thulium
168.93
[Xe]4f¹³6s²
6.1843

411
VB

412
¹⁷³Yb
Ytterbium
173.05
[Xe]4f¹⁴6s²
6.2542

419
VIB

420
¹⁷⁵Lu
Lutetium
174.97
[Xe]4f¹⁴5d¹6s²
5.4259

427
VIIB

428
²²⁷Ac
Actinium
(227)
[Rn]6d¹7s²
5.3802

435
IIB

436
²³²Th
Thorium
232.04
[Rn]6d²7s²
6.3067

443
IIIB

444
²³¹Pa
Protactinium
231.04
[Rn]5f²6d¹7s²
5.89

451
IVB

452
²³⁸U
Uranium
238.03
[Rn]5f³6d¹7s²
6.1941

459
VB

460
²³⁷Np
Neptunium
(237)
[Rn]5f⁴6d¹7s²
6.2695

467
VIB

468
²⁴⁴Pu
Plutonium
(244)
[Rn]5f⁶7s²
6.0258

475
VIIB

476
²⁴³Am
Americium
(243)
[Rn]5f⁷7s²
5.9738

483
IIB

484
²⁴⁷Cm
Curium
(247)
[Rn]5f⁸7s²
5.9914

491
IIIB

492
²⁴⁷Bk
Berkelium
(247)
[Rn]5f⁹7s²
6.1978

499
IVB

500
²⁵¹Cf
Californium
(251)
[Rn]5f¹⁰7s²
6.2817

507
VB

508
²⁵²Es
Einsteinium
(252)
[Rn]5f¹¹7s²
6.3676

515
VIB

516
²⁵⁷Fm
Fermium
(257)
[Rn]5f¹²7s²
6.80

523
VIIB

524
²⁵⁸Md
Mendelevium
(258)
[Rn]5f¹³7s²
6.58

531
IIB

532
²⁵⁹No
Nobelium
(259)
[Rn]5f¹⁴7s²
6.66

539
IIIB

540
²⁶⁰Lr
Lawrencium
(260)
[Rn]5f¹⁴7s²7p¹
4.96

547
IVB

548
²⁶¹La
Lanthanum
138.91
[Xe]5d¹6s²

555
VB

556
¹⁴⁰Ce
Cerium
140.12
[Xe]4f¹5d¹6s²
5.5386

563
VIB

564
¹⁴⁰Pr
Praseodymium
140.91
[Xe]4f³6s²
5.4702

571
VIIB

572
¹⁴⁴Nd
Neodymium
144.24
[Xe]4f⁴6s²
5.5280

579
IIB

580
¹⁴⁵Pm
Promethium
(145)
[Xe]4f⁵6s²
5.577

587
IIIB

588
¹⁵⁰Sm
Samarium
150.36
[Xe]4f⁶6s²
5.6437

595
IVB

596
¹⁵¹Eu
Europium
151.96
[Xe]4f⁷6s²
5.6704

603
VB

604
¹⁵⁷Gd
Gadolinium
157.25
[Xe]4f⁷5d¹6s²
6.1498

611
VIB

612
¹⁵⁸Tb
Terbium
158.93
[Xe]4f⁹6s²
5.8638

619
VIIB

620
¹⁶²Dy
Dysprosium
162.50
[Xe]4f¹⁰6s²
5.9391

627
IIB

628
¹⁶⁴Ho
Holmium
164.93
[Xe]4f¹¹6s²
6.0215

635
IIIB

636
¹⁶⁷Er
Erbium
167.26
[Xe]4f¹²6s²
6.1077

643
IVB

644
¹⁶⁸Tm
Thulium
168.93
[Xe]4f¹³6s²
6.1843

651
VB

652
¹⁷³Yb
Ytterbium
173.05
[Xe]4f¹⁴6s²
6.2542

659
VIB

660
¹⁷⁵Lu
Lutetium
174.97
[Xe]4f¹⁴5d¹6s²
5.4259

667
VIIB

668
²²⁷Ac
Actinium
(227)
[Rn]6d¹7s²
5.3802

675
IIB

676
²³²Th
Thorium
232.04
[Rn]6d²7s²
6.3067

683
IIIB

684
²³¹Pa
Protactinium
231.04
[Rn]5f²6d¹7s²
5.89

691
IVB

692
²³⁸U
Uranium
238.03
[Rn]5f³6d¹7s²
6.1941

699
VB

700
²³⁷Np
Neptunium
(237)
[Rn]5f⁴6d¹7s²
6.2695

707
VIB

708
²⁴⁴Pu
Plutonium
(244)
[Rn]5f⁶7s²
6.0258

715
VIIB

716
²⁴³Am
Americium
(243)
[Rn]5f⁷7s²
5.9738

723
IIB

724
²⁴⁷Cm
Curium
(247)
[Rn]5f⁸7s²
5.9914

731
IIIB

732
²⁴⁷Bk
Berkelium
(247)
[Rn]5f⁹7s²
6.1978

739
IVB

740
²⁵¹Cf
Californium
(251)
[Rn]5f¹⁰7s²
6.2817

747
VB

748
²⁵²Es
Einsteinium
(252)
[Rn]5f¹¹7s²
6.3676

755
VIB

756
²⁵⁷Fm
Fermium
(257)
[Rn]5f¹²7s²
6.80

763
VIIB

764
²⁵⁸Md
Mendelevium
(258)
[Rn]5f¹³7s²
6.58

771
IIB

772
²⁵⁹No
Nobelium
(259)
[Rn]5f¹⁴7s²
6.66

779
IIIB

780
²⁶⁰Lr
Lawrencium
(260)
[Rn]5f¹⁴7s²7p¹
4.96

787
IVB

788
²⁶¹La
Lanthanum
138.91
[Xe]5d¹6s²

795
VB

796
¹⁴⁰Ce
Cerium
140.12
[Xe]4f¹5d¹6s²
5.5386

803
VIB

804
¹⁴⁰Pr
Praseodymium
140.91
[Xe]4f³6s²
5.4702

811
VIIB

812
¹⁴⁴Nd
Neodymium
144.24
[Xe]4f⁴6s²
5.5280

819
IIB

820
¹⁴⁵Pm
Promethium
(145)
[Xe]4f⁵6s²
5.577

827
IIIB

828
¹⁵⁰Sm
Samarium
150.36
[Xe]4f⁶6s²
5.6437

835
IVB

836
¹⁵¹Eu
Europium
151.96
[Xe]4f⁷6s²
5.6704

843
VB

844
¹⁵⁷Gd
Gadolinium
157.25
[Xe]4f⁷5d¹6s²
6.1498

851
VIB

852
¹⁵⁸Tb
Terbium
158.93
[Xe]4f⁹6s²
5.8638

859
VIIB

860
¹⁶²Dy
Dysprosium
162.50
[Xe]4f¹⁰6s²
5.9391

867
IIB

868
¹⁶⁴Ho
Holmium
164.93
[Xe]4f¹¹6s²
6.0215

875
IIIB

876
¹⁶⁷Er
Erbium
167.26
[Xe]4f¹²6s²
6.1077

883
IVB

884
¹⁶⁸Tm
Thulium
168.93
[Xe]4f¹³6s²
6.1843

891
VB

892
¹⁷³Yb
Ytterbium
173.05
[Xe]4f¹⁴6s²
6.2542

899
VIB

900
¹⁷⁵Lu
Lutetium
174.97
[Xe]4f¹⁴5d¹6s²
5.4259

907
VIIB

908
²²⁷Ac
Actinium
(227)
[Rn]6d¹7s²
5.3802

915
IIB

916
²³²Th
Thorium
232.04
[Rn]6d²7s²
6.3067

923
IIIB

924
²³¹Pa
Protactinium
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[Rn]5f²6d¹7s²
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931
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932
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²³⁷Np
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955
VIIB

956
²⁴³Am
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[Rn]5f⁷7s²
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963
IIB

964
²⁴⁷Cm
Curium
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[Rn]5f⁸7s²
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971
IIIB

972
²⁴⁷Bk
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988
²⁵²Es
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[Rn]5f¹¹7s²
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995
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1003
VIIB

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1011
IIB

1012
²⁵⁹No
Nobelium
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1019
IIIB

1020
²⁶⁰Lr
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VIB

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VIIB

1052
¹⁴⁴Nd
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144.24
[Xe]4f⁴6s²
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IVB

1076
¹⁵¹Eu
Europium
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[Xe]4f⁷6s²
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1083
VB

1084
¹⁵⁷Gd
Gadolinium
157.25
[Xe]4f⁷5d¹6s²
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1091
VIB

1092
¹⁵⁸Tb
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Dysprosium
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¹⁶⁴Ho
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IIIB

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¹⁶⁷Er
Erbium
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IVB

1124
¹⁶⁸Tm
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1131
VB

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¹⁷³Yb
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VIB

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¹⁷⁵Lu
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VIIB

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IIB

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²³²Th
Thorium
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[Rn]6d²7s²
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IIIB

1164
²³¹Pa
Protactinium
231.04
[Rn]5f²6d¹7s²
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1171
IVB

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²³⁸U
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VB

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[Rn]5f⁶7s²
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VIIB

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Americium
(243)
[Rn]5f⁷7s²
5.9738

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IIB

1204
²⁴⁷Cm
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1220
²⁵¹Cf
Californium
(251)
[Rn]5f¹⁰7s²
6.2817

1227
VB

1228
²⁵²Es
Einsteinium

In this discussion, we focus our attention on the multiplet structures of atoms in their ground states, where the zero order structure is described in terms of the single particle Hamiltonian. For this discussion, the single particle Hamiltonian is a H-like ion with nuclear charge Z . As you can imagine, the numerical errors increase as Z increases. However, the qualitative features remain correct. The numerics can be improved by defining other single particle Hamiltonians. For example, density functional Hamiltonians work quite well in this context.

DEFINITION: Closed shell configuration means that for any given “shell” with orbital angular momentum quantum number l , there are $2(2l+1)$ electrons occupying that shell. For example: ns^2 np^6 nd^{10} nf^{14}

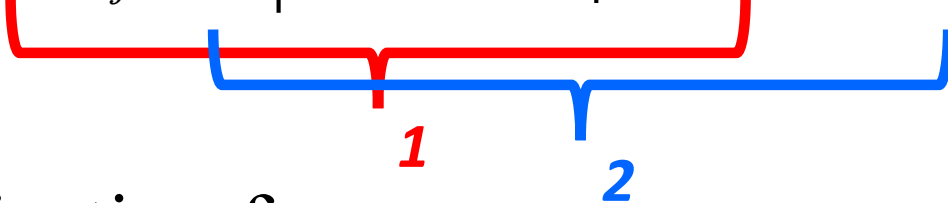
General form Hamiltonian for N -electron atom

$$H(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \sum_{i=1}^N h(\mathbf{r}_i) + V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

$$\text{where: } V(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \sum_{i=1}^N \sum_{j=1, (i>j)}^N v(\mathbf{r}_i - \mathbf{r}_j)$$

Single particle basis: $h(\mathbf{r})\varphi_k(\mathbf{r}) = \varepsilon_k \varphi_k(\mathbf{r})$

Matrix elements for electron interaction potential

$$v_{ijkl} \equiv \left\langle \varphi_i(\mathbf{r}_1) \varphi_j(\mathbf{r}_2) \left| v(\mathbf{r}_1 - \mathbf{r}_2) \right| \varphi_k(\mathbf{r}_1) \varphi_l(\mathbf{r}_2) \right\rangle$$


Hamiltonian in second quantization form:

$$H = \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

Review of ground state of He atom (example of closed shell system)

The Hamiltonian for an He atom ($Z=2$): (cgs Gaussian units)

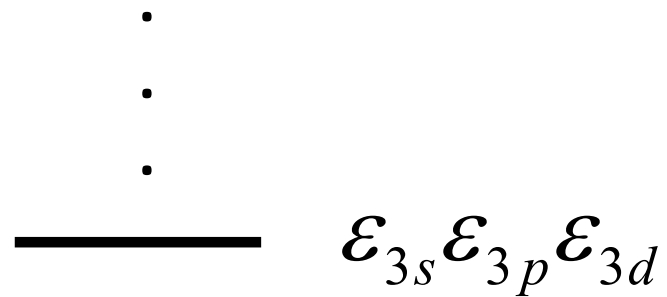
$$\begin{aligned} H(\mathbf{r}_1, \mathbf{r}_2) &= -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \\ &= -\frac{\hbar^2 \nabla_1^2}{2m} - \frac{2e^2}{r_1} - \frac{\hbar^2 \nabla_2^2}{2m} - \frac{2e^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \\ &= h(\mathbf{r}_1) + h(\mathbf{r}_2) + v(\mathbf{r}_1, \mathbf{r}_2) \end{aligned}$$

Single particle basis:

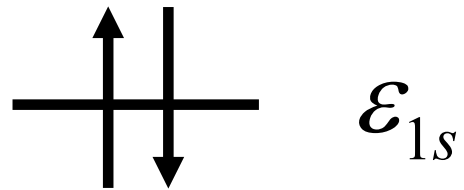
$$h(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) \equiv h(\mathbf{r}_1)\varphi_{nlmm_s}(\mathbf{r}_1) = \varepsilon_n \varphi_{nlmm_s}(\mathbf{r}_1)$$



Ground state configuration for He atom



$$\psi = f_{1s\alpha}^\dagger f_{1s\beta}^\dagger |0\rangle$$





Summary of results

$$H = \sum_i \varepsilon_i f_i^\dagger f_i + \sum_{ijkl} v_{ijkl} f_i^\dagger f_j^\dagger f_l f_k$$

Need to evaluate $\langle \psi | H | \psi \rangle$ for $\psi = f_{1s\alpha}^\dagger f_{1s\beta}^\dagger |0\rangle$

$$\langle \psi | H | \psi \rangle = 2\varepsilon_{1s} + v_{1s1s1s1s}$$

Note that in coordinate and spin representation,

$$\psi = \frac{1}{\sqrt{2}} \varphi_{1s}(\mathbf{r}_1) \varphi_{1s}(\mathbf{r}_2) (\alpha_1 \beta_2 - \alpha_2 \beta_1)$$



Example from NIST

NIST Atomic Spectra Database Levels Data

He I 198 Levels Found

$Z = 2$, He isoelectronic sequence

Configuration	Term	J	Level (eV)
$1s^2$	$1S$	0	0.00000000
$1s2s$	$3S$	1	[19.81961468]
$1s2s$	$1S$	0	[20.61577496]
$1s2p$	$3P^\circ$	2	[20.96408703]
		1	[20.96409651]
		0	[20.96421899]
$1s2p$	$1P^\circ$	1	[21.21802284]

https://physics.nist.gov/PhysRefData/ASD/levels_form.html

Example of atom with one electron outside complete shell

NIST Atomic Spectra Database Levels Data

Li I 182 Levels Found

$Z = 3$, Li isoelectronic sequence

Data on Landé factors and level compositions are not available for this ion in ASD

Some data for neutral and singly-charged ions are available in the [Handbook of Basic Atomic Spectroscopic Data](#)

Primary data source

Unpublished level list prepared for line classifications published in [Kelly 1987](#)

These data are not critically evaluated by NIST

Configuration	Term	J	Level (eV)	Uncertainty (eV)	Reference
$1s^2 2s$	2S	$1/2$	0.000000	0.000012	L3462
$1s^2 2p$	$^2P^\circ$	$1/2$	1.847818	0.000012	
		$3/2$	1.847860	0.000012	
$1s^2 3s$	2S	$1/2$	3.373129	0.000012	
$1s^2 3p$	$^2P^\circ$	$3/2$	3.834258	0.000012	

In order to analyze these atoms – we need to be able to evaluate the electron interactions

Electron-electron Coulomb repulsion:

$$v(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = e^2 \sum_{\lambda\mu} \frac{4\pi}{2\lambda + 1} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} Y_{\lambda\mu}(\hat{\mathbf{r}}_1) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_2)$$

$$\text{Define: } \mathcal{R}^\lambda(n_a l_a, n_b l_b; n_c l_c, n_d l_d) = \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} R_{n_a l_a}(r_1) R_{n_b l_b}(r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2)$$

$$\begin{aligned} v_{abcd} &\equiv \langle \varphi_a(\mathbf{r}_1) \varphi_b(\mathbf{r}_2) | v(\mathbf{r}_1 - \mathbf{r}_2) | \varphi_c(\mathbf{r}_1) \varphi_d(\mathbf{r}_2) \rangle \\ &= \sum_{\lambda\mu} \frac{e^2}{2\lambda + 1} \mathcal{R}^\lambda(n_a l_a, n_b l_b; n_c l_c, n_d l_d) G(l_a \bar{m}_a, \lambda \bar{\mu}, l_c m_c) G(l_b \bar{m}_b, \lambda \mu, l_d m_d) (-1)^{m_a + \mu + m_b} \end{aligned}$$



**These angular terms have been tabulated by
Condon and Shortley and others**

Here, the angular integrals are given in terms of Gaunt Coefficients and 3j symbols:

$$\begin{aligned} & \int_0^{2\pi} \int_0^\pi Y_{l_1, m_1}(\theta, \phi) Y_{l_2, m_2}(\theta, \phi) Y_{l_3, m_3}(\theta, \phi) \sin \theta \, d\theta \, d\phi \\ &= \left(\frac{(2l_1 + 1)(2l_2 + 1)(2l_3 + 1)}{4\pi} \right)^{\frac{1}{2}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ &\equiv \frac{1}{\sqrt{4\pi}} G(l_1 m_1, l_2 m_2, l_3 m_3) \end{aligned}$$

Note that $Y_{lm}^*(\theta, \varphi) = (-1)^m Y_{l-m}(\theta, \varphi)$

Digression on angular relationships --

“Addition” of angular momentum

Clebsch-Gordan coefficients

$$|JM, j_1 j_2\rangle = \sum_{m_1, m_2} |j_1 m_1, j_2 m_2\rangle \langle j_1 m_1, j_2 m_2 | JM, j_1 j_2\rangle$$

A more symmetric coefficient is the so-called 3-j symbol:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

Clebsch-Gordan

3-j

$$\begin{pmatrix} j_1 & m_1 & j_2 & m_2 & | & j_1 & j_2 & j_3 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 + m_3} (2j_3 + 1)^{\frac{1}{2}} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix}$$

link to more information: <http://dlmf.nist.gov/34.1>

Some symmetry properties of 3-j symbols:

$$|j_r - j_s| \leq j_t \leq j_r + j_s,$$

$$m_1 + m_2 + m_3 = 0.$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix},$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix}.$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix},$$

Some orthogonality properties of 3-j symbols:

$$\sum_{m_1 m_2} (2j_3 + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} = \delta_{j_3, j'_3} \delta_{m_3, m'_3},$$

$$\sum_{j_3 m_3} (2j_3 + 1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m_3 \end{pmatrix} = \delta_{m_1, m'_1} \delta_{m_2, m'_2},$$

$$\sum_{m_1 m_2 m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = 1.$$

Relationship of 3-j symbols to integrals over spherical harmonics and related functions

$$\int_0^\pi P_{l_1}(\cos \theta) P_{l_2}(\cos \theta) P_{l_3}(\cos \theta) \sin \theta \, d\theta = 2 \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix}^2,$$

Gaunt Coefficient

$$\begin{aligned} & \int_0^{2\pi} \int_0^\pi Y_{l_1, m_1}(\theta, \phi) Y_{l_2, m_2}(\theta, \phi) Y_{l_3, m_3}(\theta, \phi) \sin \theta \, d\theta \, d\phi \\ &= \left(\frac{(2l_1 + 1)(2l_2 + 1)(2l_3 + 1)}{4\pi} \right)^{\frac{1}{2}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \\ &\equiv \frac{1}{\sqrt{4\pi}} G(l_1 m_1, l_2 m_2, l_3 m_3) \end{aligned}$$

Explicit formula for Clebsch-Gordon coefficients:

Reference: Abramowitz & Stegun – pg. 1006

Original formula:

$$\begin{aligned} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle &= \delta_{m, m_1 + m_2} \sqrt{\frac{(j_1 + j_2 - j)! (j_1 - j_2 + j)! (-j_1 + j_2 + j)! (2j + 1)}{(j_1 + j_2 + j + 1)!}} \\ &\times \sum_k \frac{(-1)^k \sqrt{(j_1 + m_1)! (j_1 - m_1)! (j_2 + m_2)! (j_2 - m_2)! (j + m)! (j - m)!}}{k! (j_1 + j_2 - j - k)! (j_1 - m_1 - k)! (j_2 + m_2 - k)! (j - j_2 + m_1 + k)! (j - j_1 - m_2 + k)!} \end{aligned}$$

Working formula:

$$\begin{aligned} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle &= \delta_{m, m_1 + m_2} \sqrt{\frac{(j_1 - j_2 + j)! (-j_1 + j_2 + j)! (2j + 1)}{(j_1 + j_2 - j)! (j_1 + j_2 + j + 1)!}} \\ &\times \sqrt{\frac{(j_1 + m_1)! (j_2 - m_2)! (j + m)!}{(j_1 - m_1)! (j_2 + m_2)! (j - m)!}} \\ &\times \sum_k \frac{(-1)^k}{k!} \frac{(j_1 + j_2 - j)!}{(j_1 + j_2 - j - k)!} \frac{(j_1 - m_1)!}{(j_1 - m_1 - k)!} \frac{(j_2 + m_2)!}{(j_2 + m_2 - k)!} \frac{(j - m)!}{(j - j_2 + m_1 + k)! (j - j_1 - m_2 + k)!} \end{aligned}$$

Coupling of orbital angular momenta of multiple electrons

$$\mathbf{J} = \mathbf{L}_1 + \mathbf{L}_2$$

$$J = |l_1 - l_2|, |l_1 - l_2| + 1, \dots, (l_1 + l_2)$$

Example: $l_1 = l_2 = 1$ total of 9 orbital states

$J = 0$ 1 state

$J = 1$ 3 states

$J = 2$ 5 states

Consequences of orbital coupling on energies of multi-electron atoms

Example C $1s^2 2s^2 2p^2$

https://physics.nist.gov/PhysRefData/ASD/levels_form.html

Primary data source Query NIST Bibliographic Database for C I (new window)	
Moore 1993	Literature on C I Energy Levels

Configuration	Term	J	Level (eV)	Reference
$2s^2 2p^2$	3P	0	0.00000	L7288
		1	0.002033	
		2	0.005381	
$2s^2 2p^2$	1D	2	1.263725	
$2s^2 2p^2$	1S	0	2.684011	

Atomic term notation: $(2S+1)L_J$

**For the example of the single particle configuration
 np^2**

L	<i>symbol</i>	<i>spin for 2 electrons</i>
0	S	$S=0$
1	P	$S=1$
2	D	$S=0$



**In this case, it happens that $L+S=\text{even}$
why?**

Example for C $1s^2 2s^2 2p^2$

States of total orbital momentum: $(2l_1 + 1)(2l_2 + 1) = 9$

Total number of orbital and spin configurations: $6 \cdot 5 / 2 = 15$

$^1D \Rightarrow 5$ states

$^1S \Rightarrow 1$ states

$^3P \Rightarrow 9$ states

Energetic differences are due to the
electron-electron Coulomb repulsion:

$$v(\mathbf{r}_1 - \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = e^2 \sum_{\lambda\mu} \frac{4\pi}{2\lambda + 1} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} Y_{\lambda\mu}(\hat{\mathbf{r}}_1) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_2)$$

Example for 1D state

$$\begin{aligned} |JM; l_1 l_2\rangle &= |22; 11\rangle = \sum_{m_1, m_2} |l_1 m_1, l_2 m_2\rangle \langle l_1 m_1, l_2 m_2 | JM; l_1 l_2\rangle \\ &= |11, 11\rangle = R_{2p}(r_1) R_{2p}(r_2) Y_{11}(\hat{\mathbf{r}}_1) Y_{11}(\hat{\mathbf{r}}_2) \end{aligned}$$

Need to evaluate: $\langle 11, 11 | V_{ee} | 11, 11 \rangle$

where
$$V_{ee} = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = e^2 \sum_{\lambda\mu} \frac{4\pi}{2\lambda + 1} \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} Y_{\lambda\mu}(\hat{\mathbf{r}}_1) Y_{\lambda\mu}^*(\hat{\mathbf{r}}_2)$$

Define: $\mathcal{R}^\lambda(n_a l_a, n_b l_b; n_c l_c, n_d l_d)$

$$= \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}} R_{n_a l_a}(r_1) R_{n_b l_b}(r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2)$$

$$\begin{aligned} \langle 11,11 | V_{ee} | 11,11 \rangle = & e^2 \mathcal{R}^0(2p,2p;2p,2p) G^2(1-1,00,11) \\ & + e^2 \mathcal{R}^2(2p,2p;2p,2p) \frac{G^2(1-1,20,11)}{5} \end{aligned}$$

$$E(D) = e^2 \left(\mathcal{R}^0(2p,2p;2p,2p) + \frac{1}{25} \mathcal{R}^2(2p,2p;2p,2p) \right)$$

Similarly, can show that:

$$E(P) = e^2 \left(\mathcal{R}^0(2p,2p;2p,2p) - \frac{5}{25} \mathcal{R}^2(2p,2p;2p,2p) \right)$$

$$E(S) = e^2 \left(\mathcal{R}^0(2p,2p;2p,2p) + \frac{10}{25} \mathcal{R}^2(2p,2p;2p,2p) \right)$$

Summary of results:

$$\mathcal{R}^{\lambda}(n_a l_a, n_b l_b; n_c l_c, n_d l_d)$$

$$= \int_0^{\infty} r_1^2 dr_1 \int_0^{\infty} r_2^2 dr_2 \frac{r_{<}^{\lambda}}{r_{>}^{\lambda+1}} R_{n_a l_a}(r_1) R_{n_b l_b}(r_2) R_{n_c l_c}(r_1) R_{n_d l_d}(r_2)$$

$$\mathcal{R}^{\lambda}(2p, 2p; 2p, 2p)$$

$$= \int_0^{\infty} r_1^2 dr_1 R_{2p}^2(r_1) \left(\int_0^{r_1} r_2^2 dr_2 \frac{r_2^{\lambda}}{r_1^{\lambda+1}} R_{2p}^2(r_2) + \int_{r_1}^{\infty} r_2^2 dr_2 \frac{r_1^{\lambda}}{r_2^{\lambda+1}} R_{2p}^2(r_2) \right)$$

$$E(P) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) - \frac{5}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

$$E(D) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) + \frac{1}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

$$E(S) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) + \frac{10}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

Taking into account anti-symmetry of two-particle wavefunction

More details of the total angular momentum $L = 2$ case:

$$\begin{aligned} |JM; l_1 l_2\rangle &= |22; 11\rangle = \sum_{m_1, m_2} |l_1 m_1, l_2 m_2\rangle \langle l_1 m_1, l_2 m_2 | JM; l_1 l_2\rangle \\ &= |11, 11\rangle = R_{2p}(r_1) R_{2p}(r_2) Y_{11}(\hat{\mathbf{r}}_1) Y_{11}(\hat{\mathbf{r}}_2) \end{aligned}$$

Note that $\psi_D(\mathbf{r}_1, \mathbf{r}_2) = \psi_D(\mathbf{r}_2, \mathbf{r}_1)$

Full wavefunction including spin

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \sigma_1, \sigma_2) = \psi_{L=2}(\mathbf{r}_1, \mathbf{r}_2) \chi(\sigma_1, \sigma_2)$$



Must be anti-symmetric

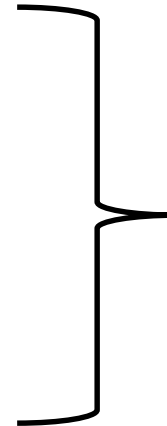
Summary of results for two spin- $\frac{1}{2}$ particle states:

$$|11; \frac{1}{2} \frac{1}{2}\rangle = |\frac{1}{2} \frac{1}{2}, \frac{1}{2} \frac{1}{2}\rangle$$

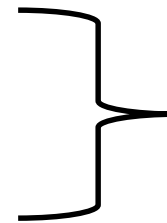
$$|10; \frac{1}{2} \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} \left(|\frac{1}{2} - \frac{1}{2}, \frac{1}{2} \frac{1}{2}\rangle + |\frac{1}{2} \frac{1}{2}, \frac{1}{2} - \frac{1}{2}\rangle \right)$$

$$|1-1; \frac{1}{2} \frac{1}{2}\rangle = |\frac{1}{2} - \frac{1}{2}, \frac{1}{2} - \frac{1}{2}\rangle$$

$$|00; \frac{1}{2} \frac{1}{2}\rangle = \frac{1}{\sqrt{2}} \left(|\frac{1}{2} - \frac{1}{2}, \frac{1}{2} \frac{1}{2}\rangle - |\frac{1}{2} \frac{1}{2}, \frac{1}{2} - \frac{1}{2}\rangle \right)$$



$S=1$, symmetric
degeneracy:
 $2S+1=3$



$S=0$,
anti-symmetric
degeneracy:
 $2S+1=1$

Extending these arguments, Condon and Shortley concluded that in general $L+S=\text{even}$

→ Valid atomic terms for Carbon:

$$(2S+1)L_J$$

$$^3P = E_0 - 5e^2\mathcal{R}^2 / 25 = 0.00 \text{ eV}$$

$$^1D = E_0 + 1e^2\mathcal{R}^2 / 25 = 1.26 \text{ eV}$$

$$^1S = E_0 + 10e^2\mathcal{R}^2 / 25 = 2.68 \text{ eV}$$

$$\Rightarrow e^2\mathcal{R}^2 / 25 \sim 0.19 \text{ eV}$$

Summary of results for analysis of atomic term energies

$$\mathcal{H} = \underbrace{\sum_i h(\mathbf{r}_i)}_{\text{single electron terms}} + \underbrace{\sum_{i,j < i} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{electron-electron interaction}}$$

Evaluating expectation values: $\langle LM | \mathcal{H} | LM \rangle$ for $2p^2$

$$E(P) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) - \frac{5}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

$$E(D) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) + \frac{1}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

$$E(S) = e^2 \left(\mathcal{R}^0(2p, 2p; 2p, 2p) + \frac{10}{25} \mathcal{R}^2(2p, 2p; 2p, 2p) \right)$$

Another example – $\text{Ti}^{+2} (1s^2 2s^2 3s^2 2p^6 3p^6 3d^2)$

Note that for simplicity, the outer $4s^2$ electrons have been removed.

From NIST:

Condon & Shortley analysis:

$${}^3F = E_0 - 8e^2 \mathcal{R}^2 / 49 - 9e^2 \mathcal{R}^4 / 441$$

$${}^1D = E_0 - 3e^2 \mathcal{R}^2 / 49 + 36e^2 \mathcal{R}^4 / 441$$

$${}^1G = E_0 + 4\mathcal{R}^2 / 49 + 1e^2 \mathcal{R}^4 / 441$$

$${}^3P = E_0 + 7e^2 \mathcal{R}^2 / 49 - 84e^2 \mathcal{R}^4 / 441$$

$${}^1S = E_0 + 14e^2 \mathcal{R}^2 / 49 + 126e^2 \mathcal{R}^4 / 441$$

Configuration	Term	J	Level (eV)
$3p^6 3d^2$	3F	2	0.0000
		3	0.02292
		4	0.05212
$3p^6 3d^2$	1D	2	1.05058
$3p^6 3d^2$	3P	0	1.30660
		1	1.31468
		2	1.32926
$3p^6 3d^2$	1G	4	1.78507
$3p^6 3d^2$	1S	0	4.02645

45 pairs of single particle states → 5 atomic terms