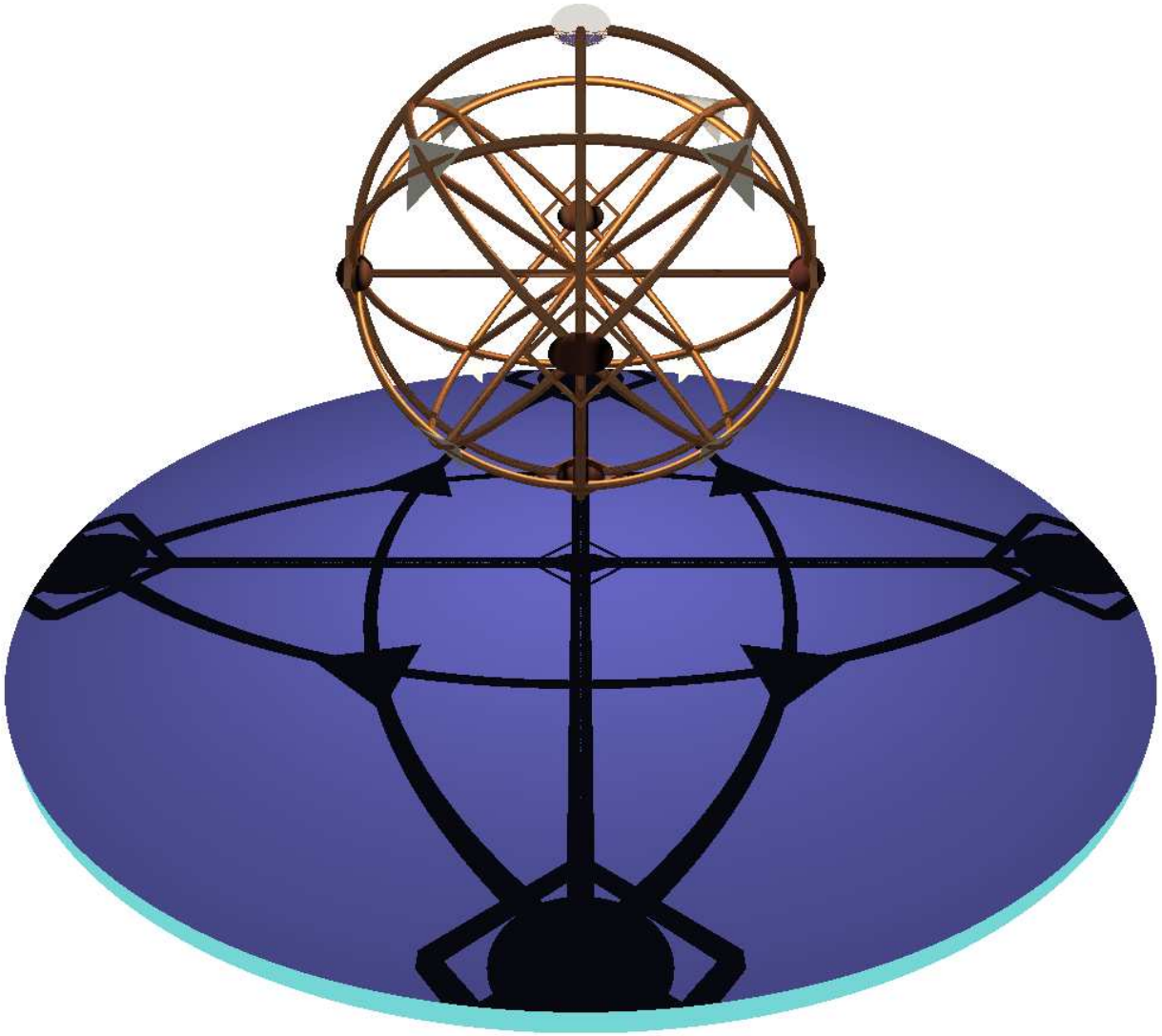
Three–Dimensional Crystals



Topics

- Distribution of structures among elements
- A small number of popular crystal structures
- Crystal symmetries:
  - 7 crystal systems
  - 14 Bravais lattices
  - 32 point groups
  - 230 space groups

The Elements

Atomic name
Atomic number and symbol
Ground state electron configuration
Melting temperature in K
Crystal structure, either at 293 K, or at melting if liquid at 293 K

SILICON u=28.09
14 Si n=4.99
$[Ne]3s^2 3p^2$
T=1683 ρ=1 · 10^5
a=5.43

Atomic weight (^{12}C=12)
Density in 10^{22} atoms cm^{-3}, at 293K or at melting
Electrical resistivity in $\mu\Omega$-cm at 298 K
Lattice parameters

Alkali Metals

Metal | Insulator | Semiconductor | Semi-metal

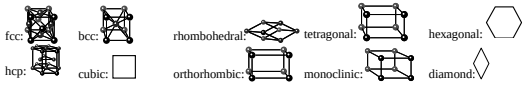
Transition Metals

Ia	IIa	IIIb	IVb	Vb	VIb	VIIb	VIIIb	VIIIb	VIIIb	Ib	IIb
LITHIUM 3 Li u=6.94 n=4.63 $1s^2 2s^1$ T=454 ρ=8.55 a=4.38	**BERYLLIUM** 4 Be u=9.01 n=12.36 $1s^2 2s^2$ T=1551 ρ=4.0 a=2.29 c=3.58										
SODIUM 11 Na u=22.99 n=2.54 $[Ne]3s^1$ T=371 ρ=4.2 a=3.77 c=6.15	**MAGNESIUM** 12 Mg u=24.31 n=4.31 $[Ne]3s^2$ T=922 ρ=4.45 a=3.21 c=5.21										
POTASSIUM 19 K u=39.10 n=1.33 $[Ar]4s^1$ T=337 ρ=6.15 a=5.33	**CALCIUM** 20 Ca u=40.08 n=2.33 $[Ar]4s^2$ T=1112 ρ=3.43 a=5.59	**SCANDIUM** 21 Sc u=44.96 n=4.00 $[Ar]3d^1 4s^2$ T=1814 ρ=61.0 a=3.31 c=5.27	**TITANIUM** 22 Ti u=47.88 n=5.70 $[Ar]3d^2 4s^2$ T=1933 ρ=42.0 a=2.95 c=4.68	**VANADIUM** 23 V u=50.94 n=7.22 $[Ar]3d^3 4s^2$ T=2160 ρ=24.8 a=3.02	**CHROMIUM** 24 Cr u=52.00 n=8.32 $[Ar]3d^5 4s^1$ T=2130 ρ=12.7 a=2.88	**MANGANESE** 25 Mn u=54.94 n=8.15 $[Ar]3d^5 4s^2$ T=1517 ρ=185.0 a=8.91	**IRON** 26 Fe u=55.85 n=8.48 $[Ar]3d^6 4s^2$ T=1808 ρ=9.71 a=2.87	**COBALT** 27 Co u=58.93 n=9.09 $[Ar]3d^7 4s^2$ T=1768 ρ=6.24 a=3.54	**NICKEL** 28 Ni u=58.69 n=9.13 $[Ar]3d^8 4s^2$ T=1726 ρ=6.84 a=3.52
RUBIDIUM 37 Rb u=85.47 n=1.08 $[Kr]5s^1$ T=312 ρ=12.5 a=5.62	**STRONTIUM** 38 Sr u=87.62 n=1.75 $[Kr]5s^2$ T=1042 ρ=23.0 a=6.08	**YTTRIUM** 39 Y u=88.91 n=3.03 $[Kr]4d^1 5s^2$ T=1795 ρ=57.0 a=3.65 c=5.73	**ZIRCONIUM** 40 Zr u=91.22 n=4.30 $[Kr]4d^2 5s^2$ T=2125 ρ=42.1 a=3.23 c=5.15	**NIOBIUM** 41 Nb u=92.91 n=5.55 $[Kr]4d^4 5s^1$ T=2741 ρ=12.5 a=3.30	**MOLYBDENUM** 42 Mo u=95.94 n=6.41 $[Kr]4d^5 5s^1$ T=2890 ρ=5.2 a=3.15	**TECHNETIUM** 43 Tc u=98.91 n=7.00 $[Kr]4d^5 5s^2$ T=2445 ρ=22.6 a=2.74 c=4.40	**RUTHENIUM** 44 Ru u=101.07 n=7.37 $[Kr]4d^7 5s^1$ T=2583 ρ=7.6 a=2.71 c=4.28	**RHODIUM** 45 Rh u=102.91 n=7.26 $[Kr]4d^8 5s^1$ T=2239 ρ=4.51 a=3.80	**PALLADIUM** 46 Pd u=106.42 n=6.80 $[Kr]4d^{10} 5s^0$ T=1825 ρ=10.8 a=3.89
CESIUM 55 Cs u=132.91 n=0.85 $[Xe]6s^1$ T=302 ρ=20.0 a=6.14	**BARIUM** 56 Ba u=137.33 n=1.57 $[Xe]6s^2$ T=1002 ρ=50 a=5.03	**LUTETIUM** 71 Lu u=174.97 n=k3.39 $[Xe]4f^{14}5d^1 6s^2$ T=1936 ρ=79.0 a=3.50 c=5.55	**HAFNIUM** 72 Hf u=178.49 n=4.49 $[Xe]4f^{14}5d^2 6s^2$ T=2503 ρ=35.1 a=3.19 c=5.05	**TANTALUM** 73 Ta u=180.95 n=5.54 $[Xe]4f^{14}5d^3 6s^2$ T=3269 ρ=12.45 a=3.30	**TUNGSTEN [WOLFRAM]** 74 W u=183.85 n=6.32 $[Xe]4f^{14}5d^4 6s^2$ T=3680 ρ=5.65 a=3.17	**RHENIUM** 75 Re u=186.20 n=6.80 $[Xe]4f^{14}5d^5 6s^2$ T=3453 ρ=19.3 a=2.76 c=4.46	**OSMIUM** 76 Os u=190.2 n=7.15 $[Xe]4f^{14}5d^6 6s^2$ T=3327 ρ=8.12 a=2.73 c=4.32	**IRIDIUM** 77 Ir u=192.22 n=7.07 $[Xe]4f^{14}5d^7 6s^2$ T=2683 ρ=5.3 a=3.84	**PLATINUM** 78 Pt u=195.08 n=6.62 $[Xe]4f^{14}5d^{10} 6s^0$ T=2045 ρ=10.6 a=3.92
FRANCIUM 87 Fr $u\approx$223 n=? $[Rn]7s^1$ T=300 ρ=? ?	**RADIUM** 88 Ra u=226.03 $n\approx$1.33 $[Rn]7s^2$ T=973 ρ=100 a=5.15	**LAWRENCIUM** 103 Lr $u\approx$260 n=? $[Rn]5f^{14}6d^1 7s^2$ T=? ρ=? ?	**RUTHERFORDIUM** 104 Rf	**DUBNIUM** 105 Db	**SEABORGIUM** 106 Sg	**BOHRIUM** 107 Bh	**HASSIUM** 108 Hs	**MEITNERIUM** 109 Mt			

Lanthanides [Rare Earths]									
LANTHANUM 57 La u=138.91 n=2.67 $[Xe]5d^1 6s^2$ T=1194 ρ=57 a=3.77 c=1.22	**CERIUM** 58 Ce u=140.12 n=3.54 $[Xe]4f^2 5d^0 6s^2$ T=1072 ρ=73 a=4.85	**PRASEODYMIUM** 59 Pr u=140.91 n=2.89 $[Xe]4f^3 5d^0 6s^2$ T=1204 ρ=68 a=3.67 c=11.83	**NEODYMIUM** 60 Nd u=144.24 n=2.93 $[Xe]4f^4 5d^0 6s^2$ T=1294 ρ=64.0 a=3.66 c=11.80	**PROMETHIUM** 61 Pm $u\approx$145 n=3.00 $[Xe]4f^5 5d^0 6s^2$ T=1441 $\rho\approx$50 a=?	**SAMARIUM** 62 Sm u=150.36 n=3.01 $[Xe]4f^6 5d^0 6s^2$ T=1350 ρ=94.0 a=9.00 α=23° 13′	**EUROPIUM** 63 Eu u=151.97 n=2.08 $[Xe]4f^7 5d^0 6s^2$ T=1095 ρ=90.0 a=4.58
ACTINIUM 89 Ac u=227.03 n=2.67 $[Rn]6d^1 7s^2$ T=1320 ρ=? a=5.31	**THORIUM** 90 Th u=232.04 n=3.04 $[Rn]5f^0 6d^2 7s^2$ T=2023 ρ=13.0 a=5.08	**PROTACTINIUM** 91 Pa u=231.04 n=4.34 $[Rn]5f^2 6d^1 7s^2$ T=2113 ρ=17.7 a=3.93 c=3.24	**URANIUM** 92 U u=238.03 n=4.79 $[Rn]5f^3 6d^1 7s^2$ T=1406 ρ=30.8 a=2.85 b=5.86 c=4.95	**NEPTUNIUM** 93 Np u=237.05 n=5.14 $[Rn]5f^4 6d^1 7s^2$ T=913 ρ=122 a=4.72 b=4.89 c=6.66	**PLUTONIUM** 94 Pu $u\approx$244 n=4.89 $[Rn]5f^6 6d^0 7s^2$ T=914 ρ=146 a=6.18 b=4.82 c=10.96 β=101° 48′	**AMERICIUM** 95 Am $u\approx$243 $n\approx$3.39 $[Rn]5f^7 6d^0 7s^2$ T=1267 ρ=68 a=3.47 c=11.24

Actinides

The Elements



						Halogens VIIa	Noble Gases VIIIa
						Hydrogen 1 H u=1.008 n=4.54 $1s^1$ T=14.01 ρ=? a=3.77 c=6.16	Helium 2 He u=4.003 n=3.11 $1s^2$ At 2 K, 26 atm a=3.53 c=4.24
		IIIa	IVa	Va	VIa		
Noble metals Ib	IIb						
		Boron 5 B u=10.81 n=13.03 $1s^2 2s^2 2p^1$ T=2573 ρ=$1.8 \cdot 10^{12}$ a=8.74 c=5.06	Carbon 6 C u=12.01 n=17.59 $1s^2 2s^2 2p^2$ T=3820 ρ=10^{19} a=3.57	Nitrogen 7 N u=14.01 n=4.43 $1s^2 2s^2 2p^3$ T=63.29 ρ=? a=5.64	Oxygen 8 O u=16.00 n=7.53 $1s^2 2s^2 2p^4$ T=54.8 ρ=? a=6.83	Fluorine 9 F u=19.00 n=? $1s^2 2s^2 2p^5$ T=53.5 ρ=? a=6.67	Neon 10 Ne u=20.18 n=4.30 $1s^2 2s^2 2p^6$ T=24.5 ρ=? a=4.45
		Aluminum 13 Al u=26.98 n=6.02 $[Ne]3s^2 3p^1$ T=934 ρ=2.65 a=4.05	Silicon 14 Si u=28.09 n=4.99 $[Ne]3s^2 3p^2$ T=1683 ρ=$1 \cdot 10^5$ a=5.43	Phosphorus 15 P u=30.97 n=3.54 $[Ne]3s^2 3p^3$ T=317 ρ=$1 \cdot 10^{17}$ a=18.51	Sulfur 16 S u=32.07 n=3.89 $[Ne]3s^2 3p^4$ T=386 ρ=$2 \cdot 10^{23}$ a=10.46 b=12.87 c=24.49	Chlorine 17 Cl u=35.45 n=3.45 $[Ne]3s^2 3p^5$ T=172 ρ=? a=6.24 b=4.48 c=8.26	Argon 18 Ar u=39.95 n=2.50 $[Ne]3s^2 3p^6$ T=83.8 ρ=? a=5.31
Copper 29 Cu u=63.55 n=8.49 $[Ar]3d^{10} 4s^1$ T=1357 ρ=1.67 a=3.61	Zinc 30 Zn u=65.39 n=6.56 $[Ar]3d^{10} 4s^2$ T=693 ρ=5.92 a=2.66 c=4.95	Gallium 31 Ga u=69.72 n=5.10 $[Ar]3d^{10} 4s^2 4p^1$ T=303 ρ=27 a=4.52 b=7.66 c=4.53	Germanium 32 Ge u=72.61 n=4.41 $[Ar]3d^{10} 4s^2 4p^2$ T=1211 ρ=$4.6 \cdot 10^7$ a=5.66	Arsenic 33 As u=74.92 n=4.64 $[Ar]3d^{10} 4s^2 4p^3$ T=1090 ρ=26 a=4.13 α=54°10′	Selenium 34 Se u=78.96 n=3.65 $[Ar]3d^{10} 4s^2 4p^4$ T=490 ρ=$1 \cdot 10^6$ a=4.37 c=4.96	Bromine 35 Br u=79.90 n=3.05 $[Ar]3d^{10} 4s^2 4p^5$ T=266 ρ=? a=6.74 b=4.55 c=8.76	Krypton 36 Kr u=83.80 n=2.03 $[Ar]3d^{10} 4s^2 4p^6$ T=117 ρ=? a=5.72
Silver 47 Ag u=107.87 n=5.86 $[Kr]4d^{10} 5s^1$ T=1235 ρ=1.59 a=4.09	Cadmium 48 Cd u=112.41 n=4.63 $[Kr]4d^{10} 5s^2$ T=594 ρ=6.83 a=2.98 c=5.62	Indium 49 In u=114.82 n=3.83 $[Kr]4d^{10} 5s^2 5p^1$ T=429 ρ=8.37 a=3.23 c=4.94	Tin 50 Sn u=118.71 n=3.71 $[Kr]4d^{10} 5s^2 5p^2$ T=505 ρ=11.0 a=5.83 c=3.18	Antimony 51 Sb u=121.75 n=3.31 $[Kr]4d^{10} 5s^2 5p^3$ T=904 ρ=39.0 a=4.51 α=57°7′	Tellurium 52 Te u=127.60 n=2.94 $[Kr]4d^{10} 5s^2 5p^4$ T=723 ρ=$4.36 \cdot 10^5$ a=4.46 c=5.93	Iodine 53 I u=126.91 n=2.34 $[Kr]4d^{10} 5s^2 5p^5$ T=387 ρ=$1.3 \cdot 10^{15}$ a=7.26 b=4.79 c=9.79	Xenon 54 Xe u=131.29 n=1.62 $[Kr]4d^{10} 5s^2 5p^6$ T=161 ρ=? a=6.19
Gold 79 Au u=196.97 n=5.90 $[Xe]4f^{14} 5d^{10} 6s^1$ T=1338 ρ=2.35 a=4.08	Mercury 80 Hg u=100.59 n=4.07 $[Xe]4f^{14} 5d^{10} 6s^2$ T=234 ρ=94.1 a=2.99 α=70°45′	Thallium 81 Tl u=204.38 n=3.49 $[Xe]4f^{14} 5d^{10} 6s^2 6p^1$ T=577 ρ=18.0 a=3.46 c=5.53	Lead 82 Pb u=207.2 n=3.30 $[Xe]4f^{14} 5d^{10} 6s^2 6p^2$ T=601 ρ=20.65 a=4.95	Bismuth 83 Bi u=208.98 n=2.81 $[Xe]4f^{14} 5d^{10} 6s^2 6p^3$ T=545 ρ=106.8 a=4.75 α=57°14′	Polonium 84 Po u≈209 n=2.68 $[Xe]4f^{14} 5d^{10} 6s^2 6p^4$ T=527 ρ=140 a=3.35	Astatine 85 At u≈210 n=? $[Xe]4f^{14} 5d^{10} 6s^2 6p^5$ T≈575 ρ=? ?	Radon 86 Rn u≈222 n=? $[Xe]4f^{14} 5d^{10} 6s^2 6p^6$ T=202 ρ=? a=?

Gadolinium 64 Gd u=157.25 n=3.02 $[Xe]4f^7 5d^1 6s^2$ T=1586 ρ=134 a=3.64	Terbium 65 Tb u=158.93 n=3.12 $[Xe]4f^9 5d^0 6s^2$ T=1629 ρ=114 a=3.59 b=6.26 c=5.72	Dysprosium 66 Dy u=162.50 n=3.17 $[Xe]4f^{10} 5d^0 6s^2$ T=1685 ρ=57.0 a=3.59 c=5.65	Holmium 67 Ho u=164.93 n=3.21 $[Xe]4f^{11} 5d^0 6s^2$ T=1747 ρ=87.0 a=3.58 c=5.62	Erbium 68 Er u=167.27 n=3.26 $[Xe]4f^{12} 5d^0 6s^2$ T=1802 ρ=87 a=3.56 c=5.59	Thulium 69 Tm u=168.93 n=3.32 $[Xe]4f^{13} 5d^0 6s^2$ T=1818 ρ=79.0 a=3.54 c=5.55	Ytterbium 70 Yb u=173.04 n=2.42 $[Xe]4f^{14} 5d^0 6s^2$ T=1097 ρ=29.0 a=5.49
Curium 96 Cm u≈247 n=3.24 $[Rn]5f^7 6d^1 7s^2$ T=1610 ρ=? ?	Berklium 97 Bk u≈247 n=3.60 $[Rn]5f^9 6d^0 7s^2$ T=? ρ= ?	Californium 98 Cf u≈251 n=? $[Rn]5f^{10} 6d^0 7s^2$ T=? ρ=? a=? ?	Einsteinium 99 Es u≈254 n=? $[Rn]5f^{11} 6d^0 7s^2$ T=? ρ=? ?	Fermium 100 Fm u≈257 n=? $[Rn]5f^{12} 6d^0 7s^2$ T=? ρ=? ?	Mendelevium 101 Md u≈258 n=? $[Rn]5f^{13} 6d^0 7s^2$ T=? ρ=? ?	Nobelium 102 No u≈259 n=? $[Rn]5f^{14} 6d^0 7s^2$ T=? ρ=? ?

Web Elements

16th May 2003

Allotropy

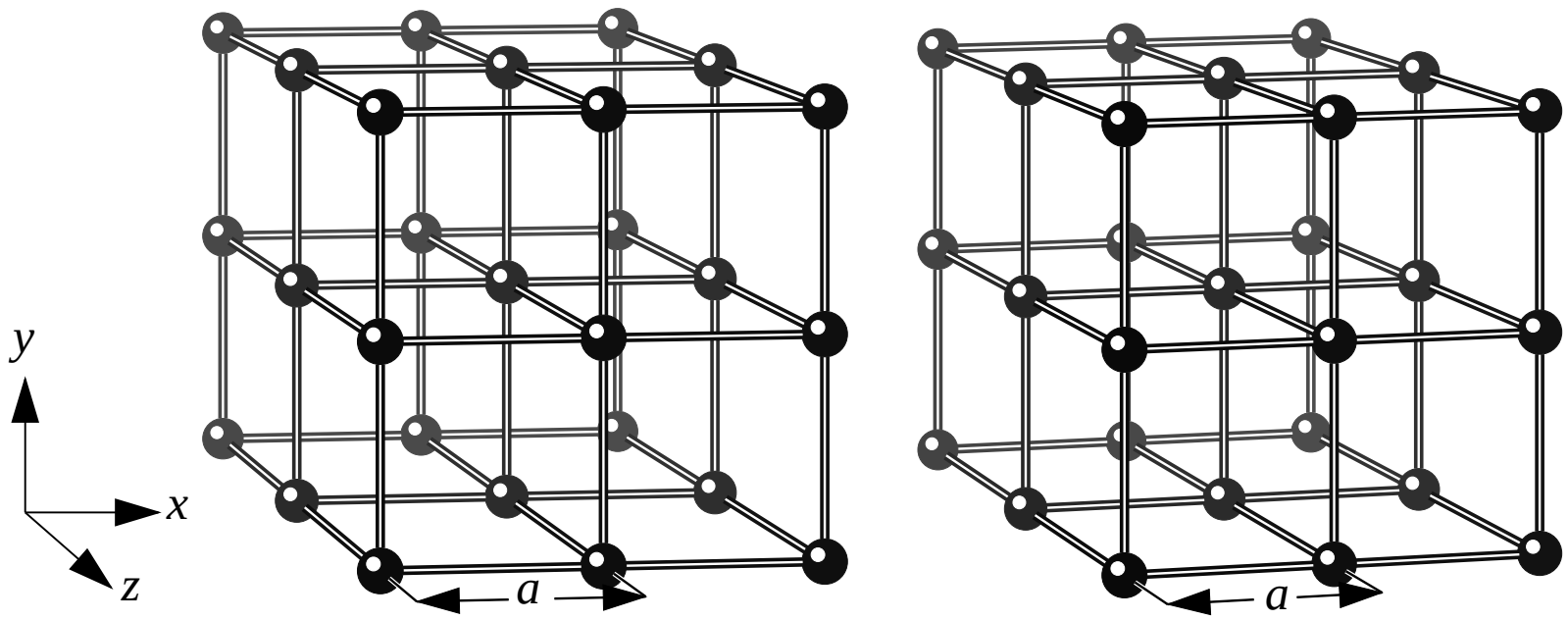
Many elements adopt multiple crystal structures between 0 K and their melting temperature. Plutonium has a particularly elaborate phase diagram:

Transformation Temp, C	Phase	Structure (atoms per unit cell)	Density (g/cc)
112	α	monoclinic (16)	19.8
185	β	fc monoclinic (34)	17.8
310	γ	fc orthorhombic (8)	17.1
450	δ	fcc (4)	15.9
475	δ'	fc tetragonal (2)	16.0
640	ϵ	bcc (2)	16.5

Table 1: Source, Atomic Weapons Establishment, Discovery Article

Popular Lattices

Simple Cubic



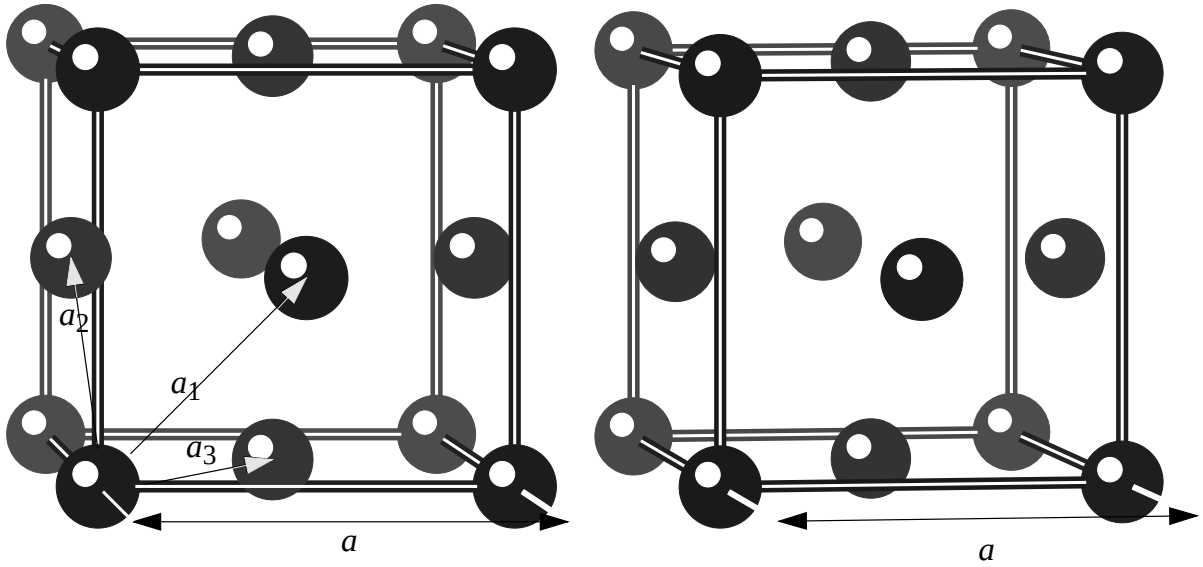
To view these crystals in 3–d, install `rasmol`. Using xpdf version 2, one can click on the name above each figure and invoke rasmol automatically. Configure rasmol with a .rasmolrc file containing

spacefill 100

wireframe 20

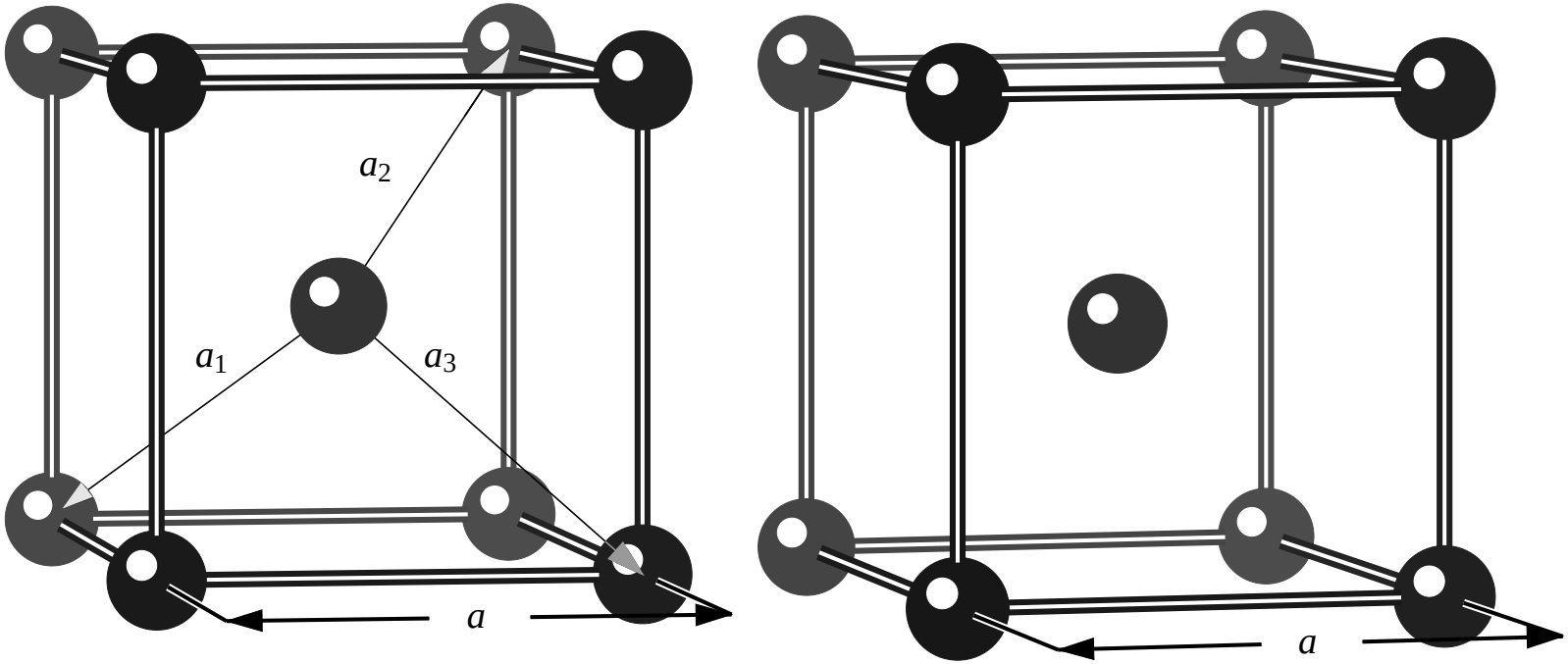
Popular Lattices

Face Centered Cubic (fcc)



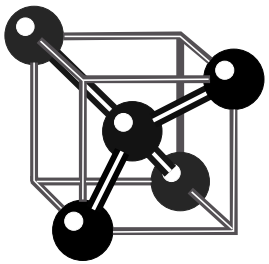
Popular Lattices

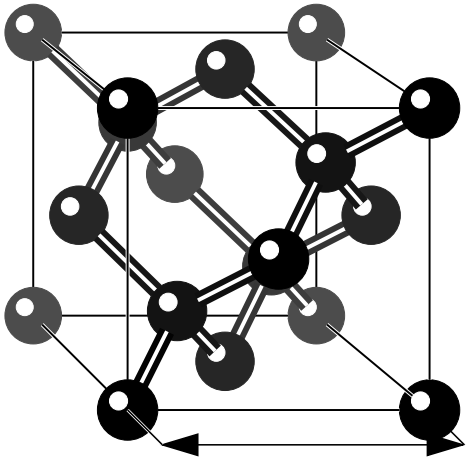
Body Centered Cubic (bcc)



Popular Lattices

Diamond





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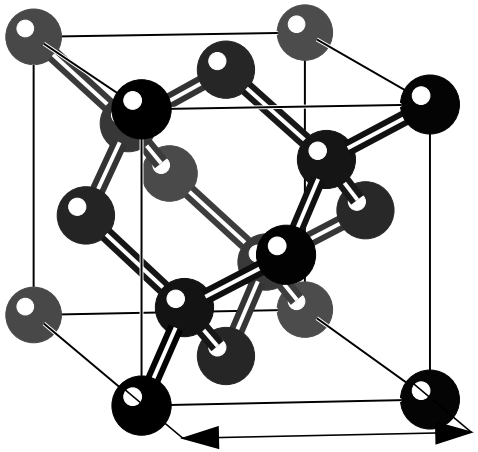

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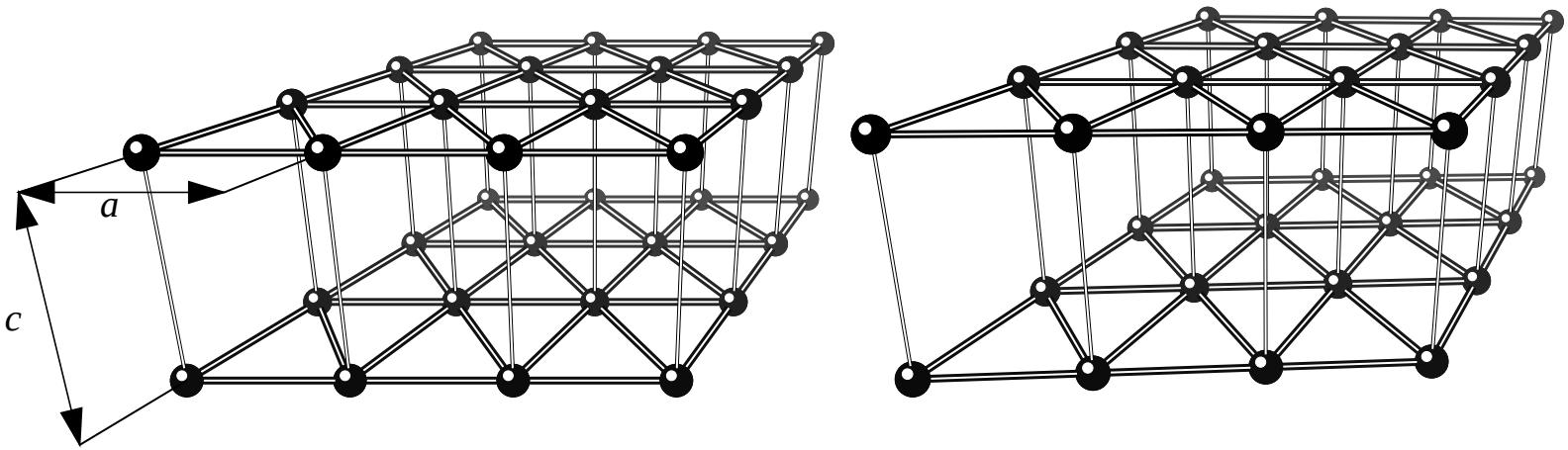
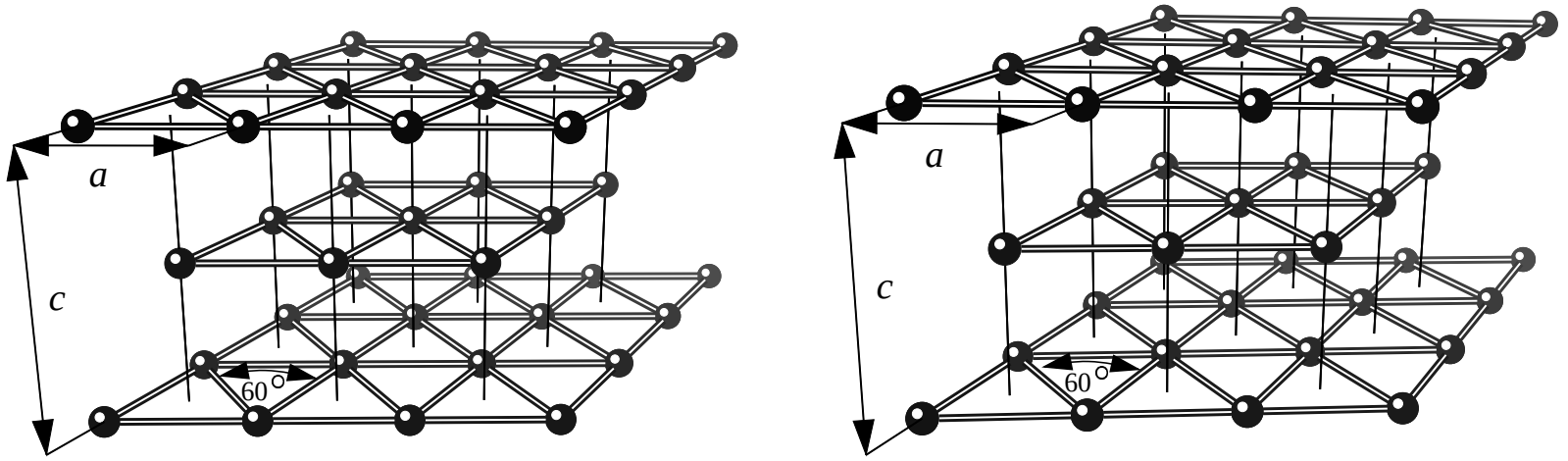
Popular Lattices

Hexagonal



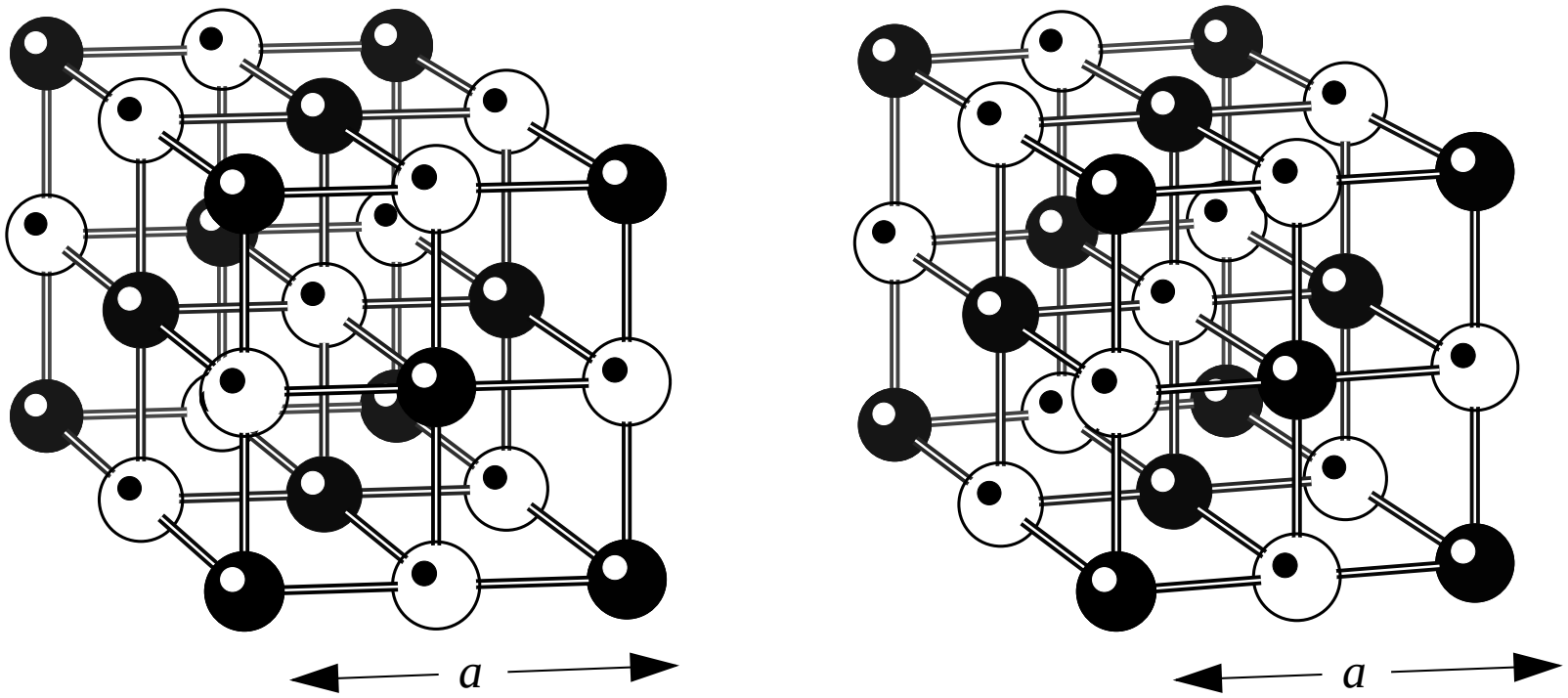
Popular Lattices

Hexagonal Close Packed (hcp)



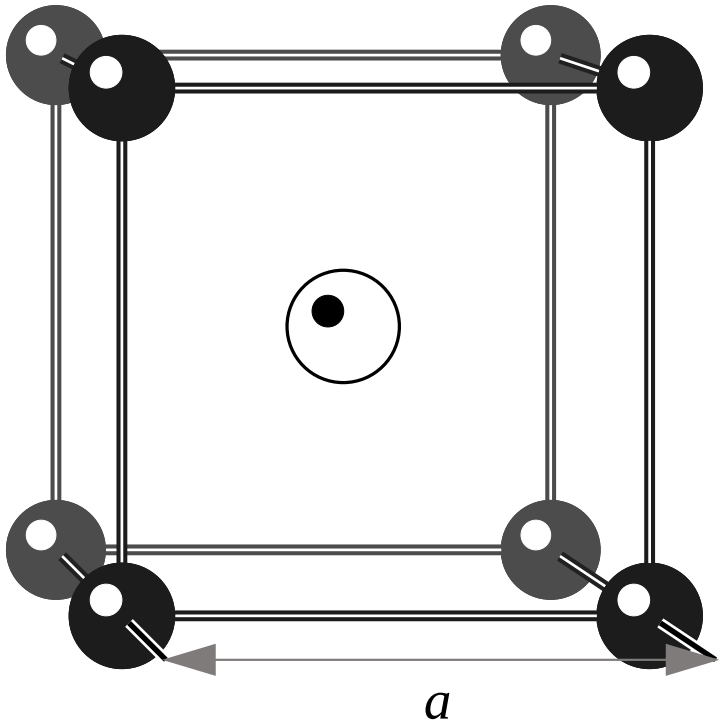
Popular Lattices

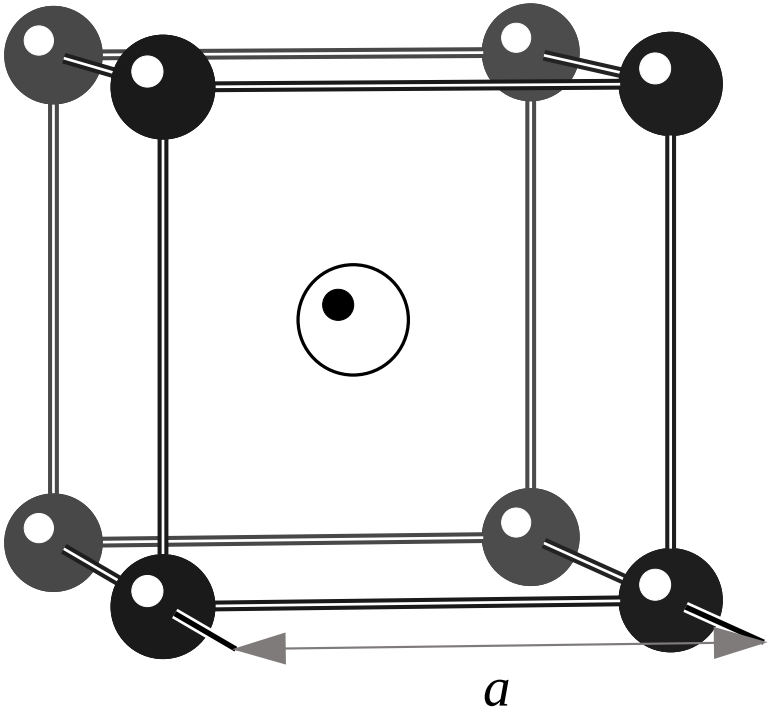
Sodium Chloride (NaCl)



Popular Lattices

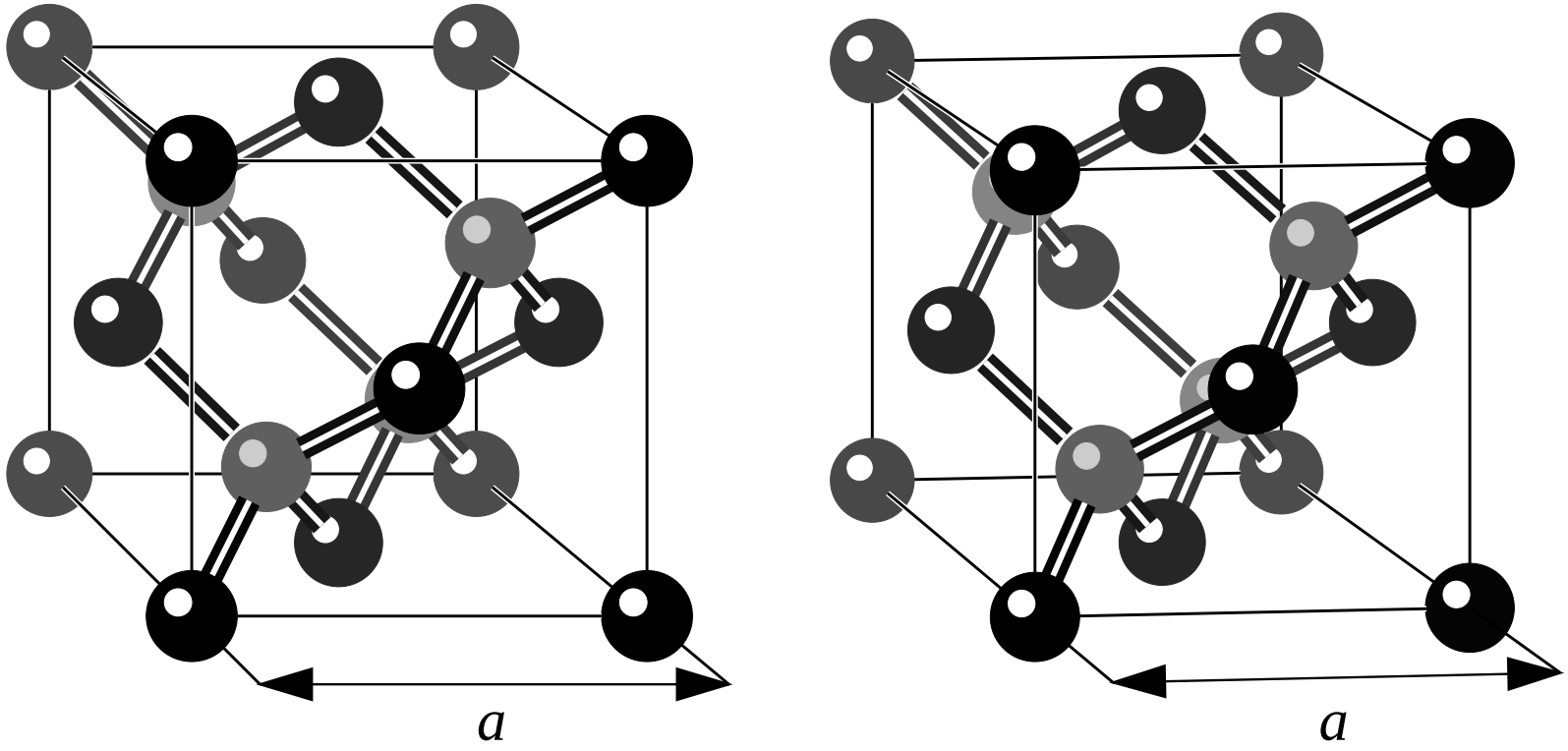
Cesium Chloride (CeCl)





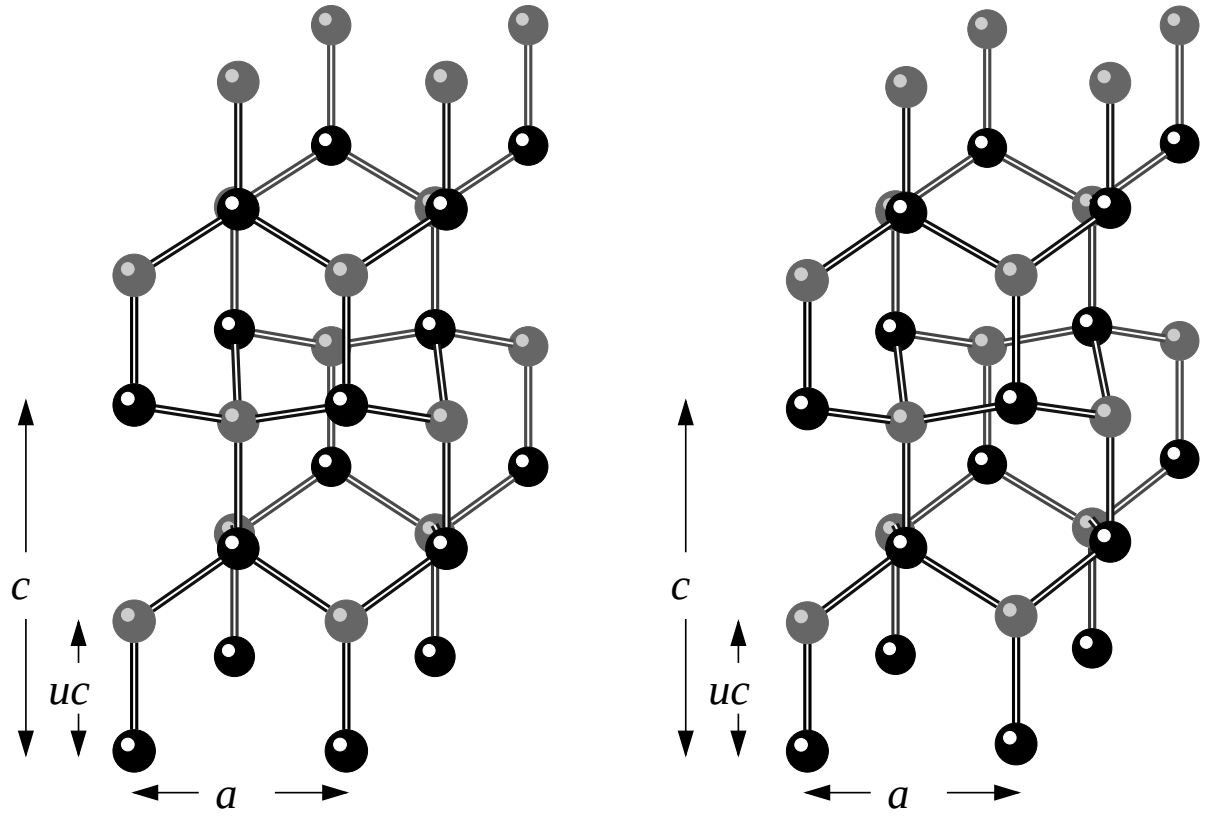
Popular Lattices

Zincblende



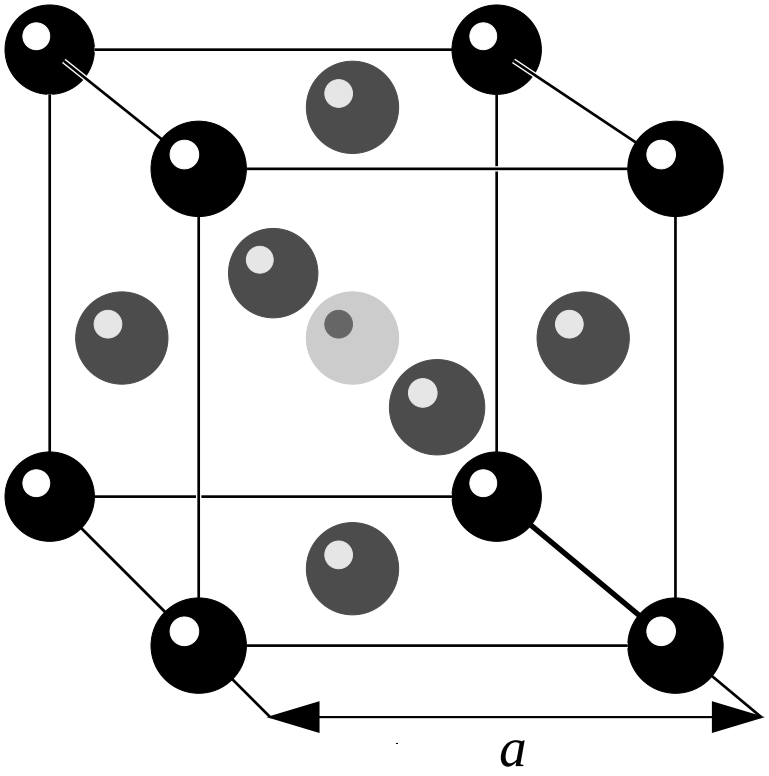
Popular Lattices

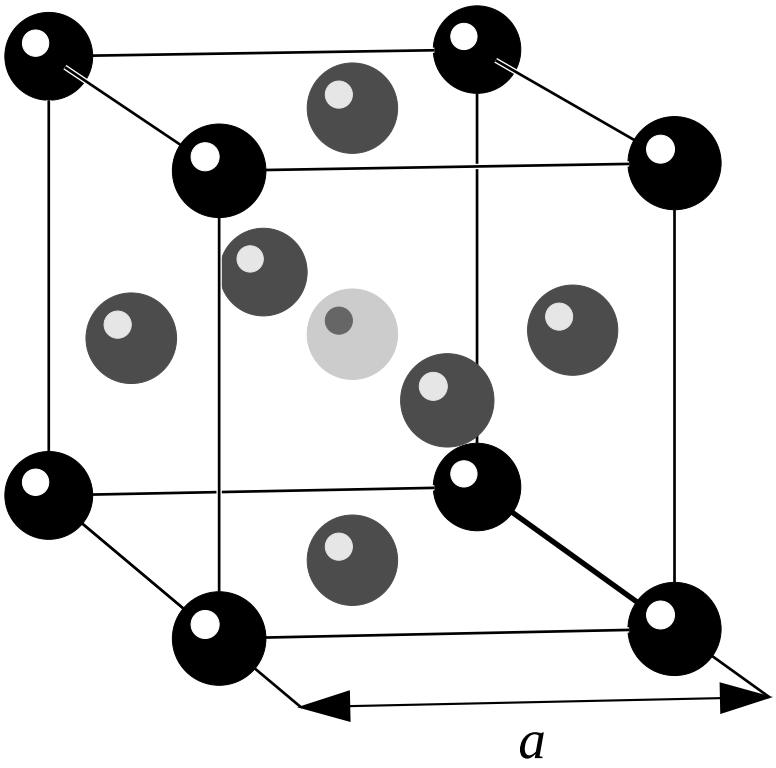
Wurtzite



Popular Lattices

Perovskite





Fourteen Bravais Lattices and Seven Crystal Systems

Please welcome The Bravais Lattice Song

http://www.haverford.edu/physics-astro/songs/bravais.htm

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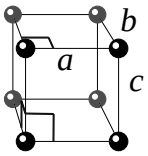
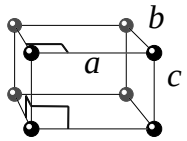
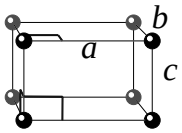
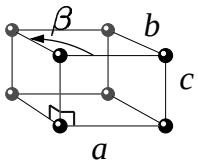
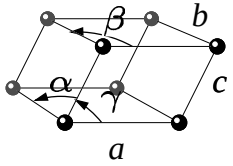
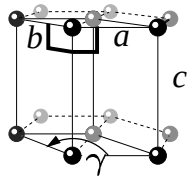
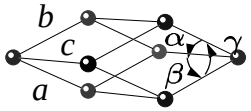
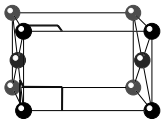
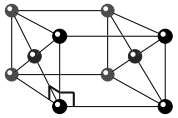
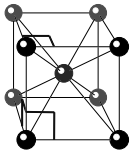
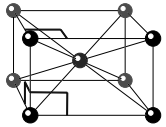
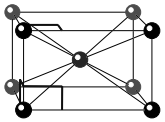
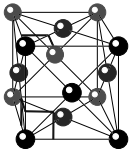
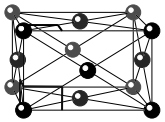
	Cubic $a=b=c$ $\alpha=\beta=\gamma=90^\circ$	Tetragonal $a=b\neq c$ $\alpha=\beta=\gamma=90^\circ$	Orthorhombic $a\neq b\neq c$ $\alpha=\beta=\gamma=90^\circ$	Monoclinic $a\neq b\neq c$ $\alpha=\gamma=90^\circ$ $\beta\neq 90^\circ$	Triclinic $a\neq b\neq c$ $\alpha,\beta,\gamma\neq 90^\circ$	Hexagonal $a=b\neq c$ $\alpha=\beta=90^\circ$ $\gamma=120^\circ$	Rhombohedral $a=b=c$ $\alpha=\beta=\gamma\neq 90^\circ$
Simple							
Base-Centered							
Body-Centered							
Face-Centered							

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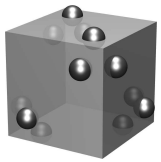
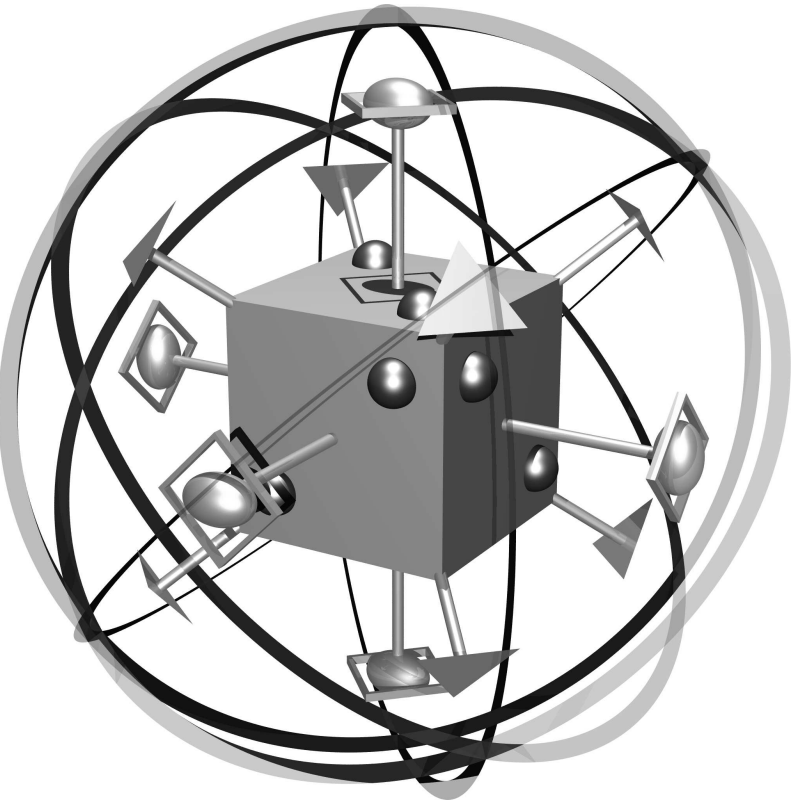
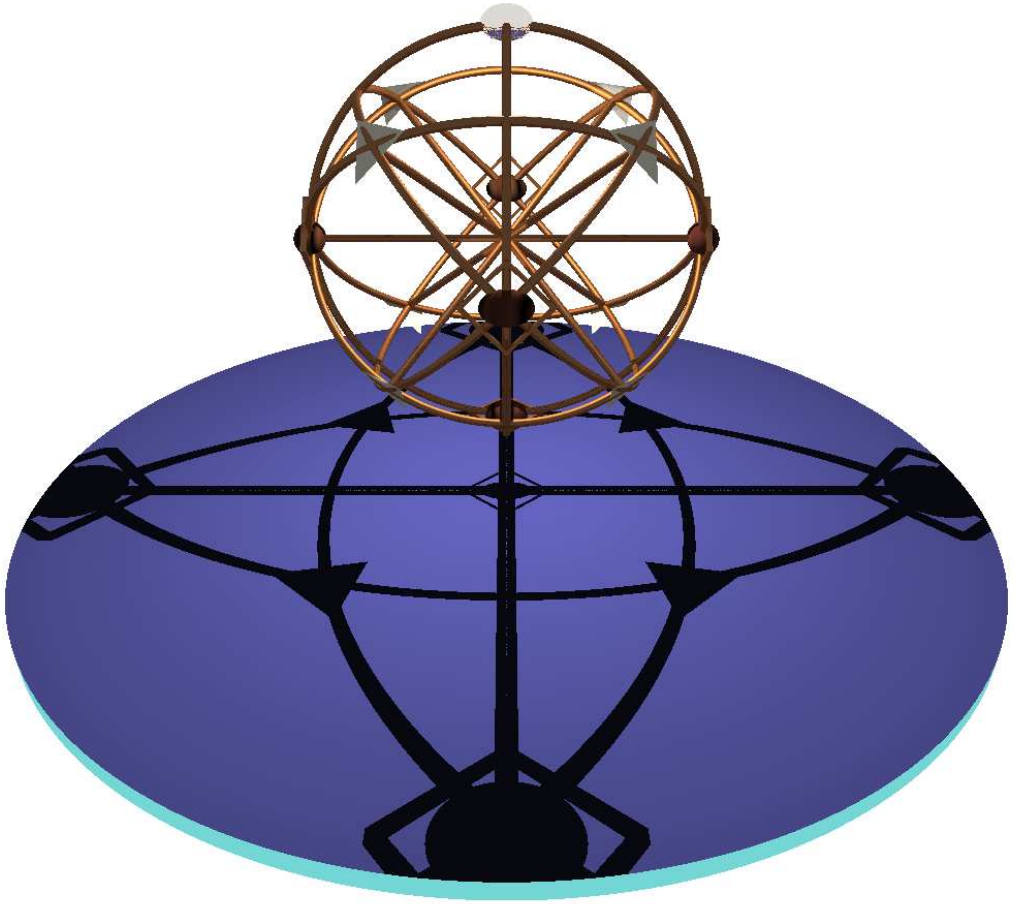






Symmetry Axes

Axis type	Schönflies Notation	International Notation	Symbol	Operation
Inversion	$i = S_2$	$\bar{1}$	○	$\vec{r} \rightarrow -\vec{r}$
Twofold	C_2	2	or	
Threefold	C_3	3	or	
Fourfold	C_4	4		
Sixfold	C_6	6		
Twofold Rotoinversion or Mirror	σ_h, $\perp$ to axis σ_v, plane contains axis σ_d, bisects twofold axes	$\bar{2} \equiv m$	or	
Threefold Rotoinversion	S_6^{-1}	$\bar{3}$		
Fourfold Rotoinversion	S_4^{-1}	$\bar{4}$		
Sixfold Rotoinversion	S_3^{-1}	$\bar{6}$		

Schönflies and international notation

Schönflies

C = Cyclic; allows successive rotation about main axis.

D = Dihedral; contains two-fold axes perpendicular to main axis.

S = Spiegel; unchanged after combination of reflection and rotation.

T = Tetragonal.

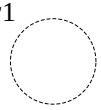
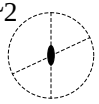
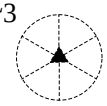
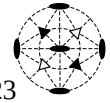
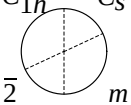
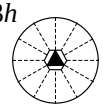
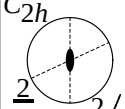
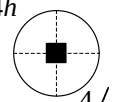
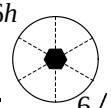
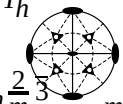
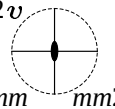
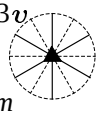
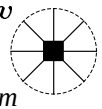
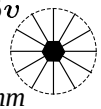
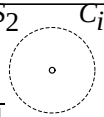
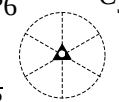
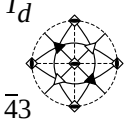
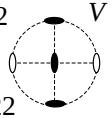
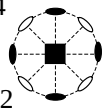
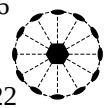
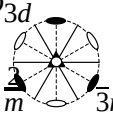
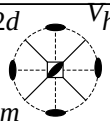
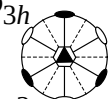
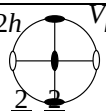
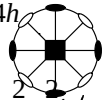
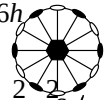
O = Octahedral.

A subscript $n = 1 \ldots 6$ denotes the order of a rotation axis, and subscripts h, v, and d denote the three types of mirror plane on previous slide.

International

Associates each group with a list of its symmetry axes Notation such as $6m$ refers to a mirror plane containing a sixfold axis, while $\frac{6}{m}$ refers to a mirror plane perpendicular to a sixfold axis.

32 Crystallographic Point Groups

Triclinic	Monoclinic	Ortho-rhombic	Trigonal	Tetragonal	Hexagonal	Cubic
C_1  1	C_2  2		C_3  3	C_4  4	C_6  6	T  23
	C_{1h} C_s  $\bar{2}$ m				C_{3h}  $\bar{6}$	
	C_{2h}  $\frac{2}{m}$ $2/m$			C_{4h}  $\frac{4}{m}$ $4/m$	C_{6h}  $\frac{6}{m}$ $6/m$	T_h  $\frac{2}{m}\bar{3}$ $m\bar{3}$
		C_{2v}  2mm mm2	C_{3v}  3m	C_{4v}  4mm	C_{6v}  6mm	
S_2 C_i  $\bar{1}$			S_6 C_{3i}  $\bar{3}$	S_4  $\bar{4}$		T_d  $\bar{4}3$
		D_2 V  222	D_3  32	D_4  422	D_6  622	O  432
			D_{3d}  $\bar{3}\frac{2}{m}$ $\bar{3}m$	D_{2d} V_h  $\bar{4}2m$		
					D_{3h}  $\bar{6}m2$	
		D_{2h} V_h  $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ mmm		D_{4h}  $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $4/mmm$	D_{6h}  $\frac{6}{m}\frac{2}{m}\frac{2}{m}$ $6/mmm$	O_h  $\frac{4}{m}\bar{3}\frac{2}{m}$ $m\bar{3}m$

230 Space Groups

Learn as much as you want at

http://cst-www.nrl.navy.mil/lattice/spcgrp/

http://www.uwgb.edu/dutchs/SYMMETRY/3dSpaceGrps/3DSPGRP.HTM

http://www-structure.llnl.gov/Xray/tutorial/spcgrps.htm

http://www.ccas.ru/galiulin/feddos1.html

Some consequences of symmetry

Sometimes it is possible to decide that some particular effect must vanish in a particular crystal simply by considering its symmetries. Magic when it works.

Example: Piezoelectricity

$$e_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial u_\alpha}{\partial r_\beta} + \frac{\partial u_\beta}{\partial r_\alpha}\right). \tag{L1}$$

$$P_\gamma = \sum_{\alpha\beta} \mathcal{B}_{\alpha\beta\gamma}\, e_{\alpha\beta}, \tag{L2}$$

$\mathcal{B}$ is the most general possible tensor describing a general linear relationship between dipole moment and the strain, and is computed by considering all atoms in equilibrium.

Consider $r \to -\vec{r}$.

Crystal cannot be centrosymmetric, ruling out possibility of (large) effect in huge numbers of compounds.