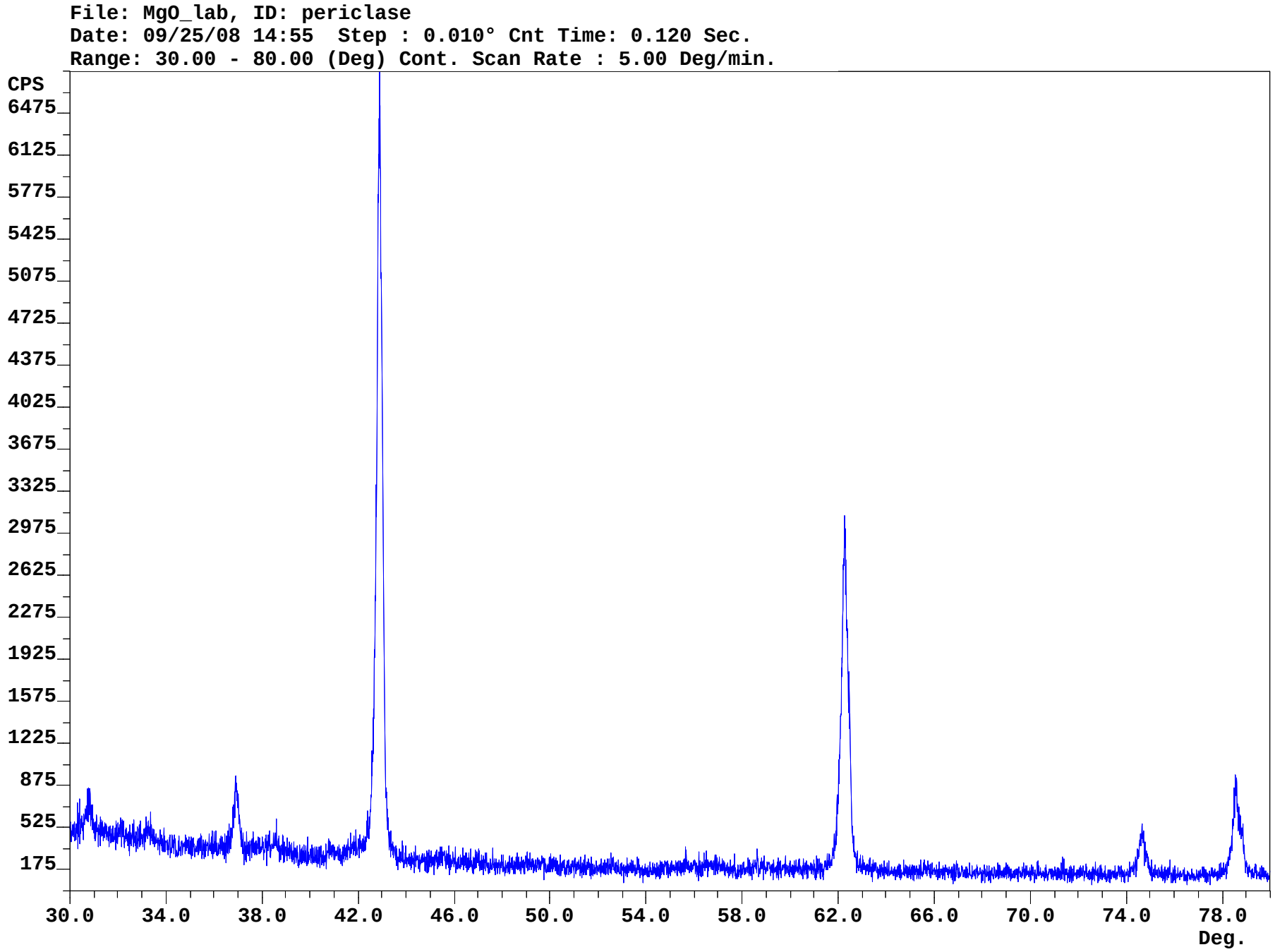

File: MgO_lab, ID: periclase
Date: 09/25/08 14:55 Step : 0.010° Cnt Time: 0.120 Sec.
Range: 30.00 - 80.00 (Deg) Cont. Scan Rate : 5.00 Deg/min.
CPS
6475
6125
5775
5425
5075
4725
4375
4025
3675
3325
2975
2625
2275
1925
1575
1225
875
525
175
30.0
34.0
38.0
42.0
46.0
50.0
54.0
58.0
62.0
66.0
70.0
74.0
78.0
Deg.

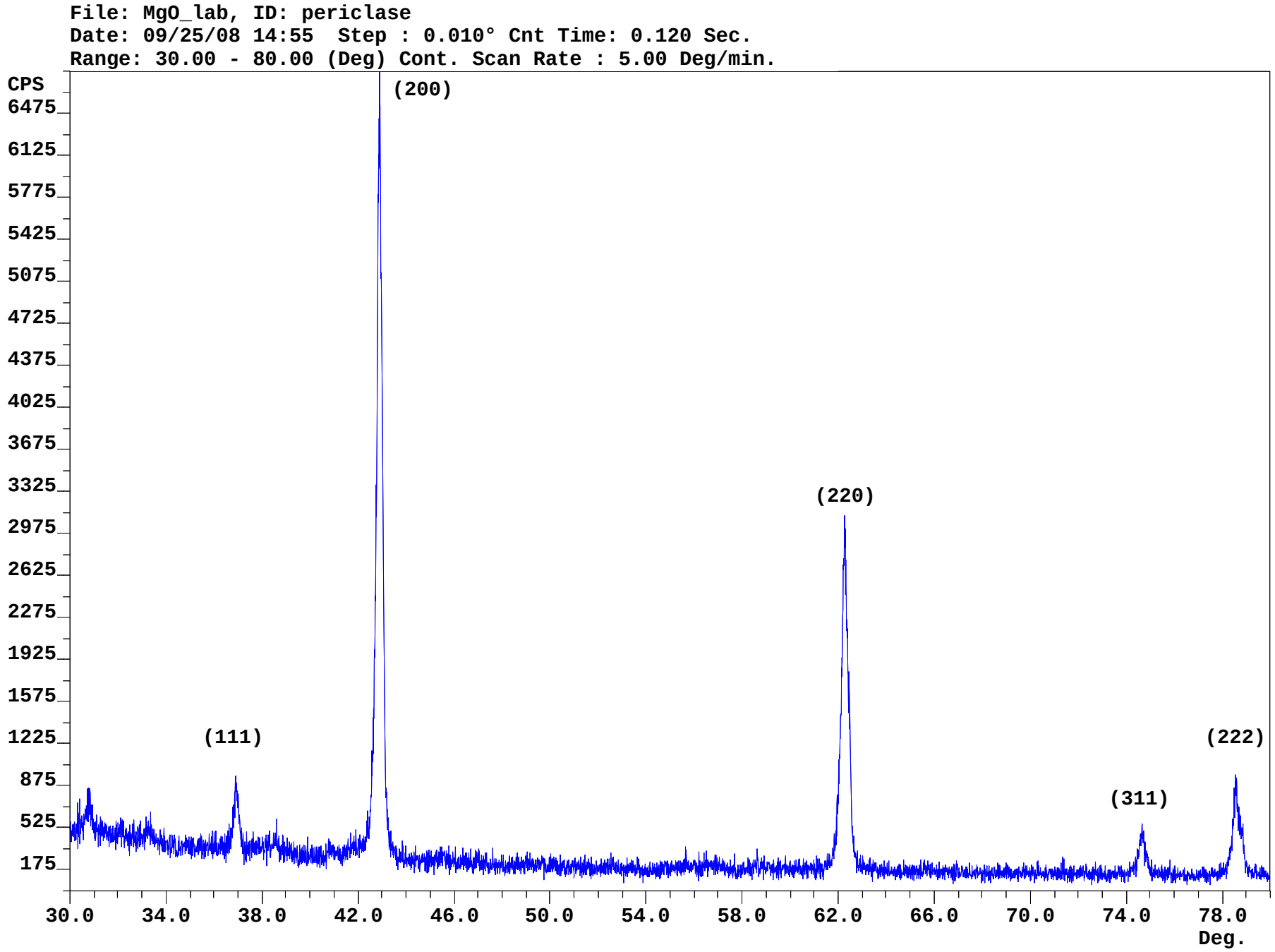
MgO
Magnesium Oxide
Periclase, Syn

Rad:CuKa1	Lambda:1.5405	Filter:Beta filter used	d sp:	
Cutoff:	Int:	I/Icor:2.1		
Ref:Swanson, Tatge., 1 37, (1953)				
Sys:Cubic		S.G.:Fm3m		
a:4.213	b:	c:		
α:	β:	γ:	Z:4	mp
Ref2				
Dx:3.581	Dm:3.58	SS/FOM: F10=55.7(0.018,10)	Volume[CD]:74.78	
εα:	ηωβ:1.732	εγ:	Sign:	2V:
Ref3				
Color:Colorless				

High purity phosphor sample from RCA heated at 1800 C for 3 hours. Pattern at 26 C. Spectrographic analysis in %: Ca and Si 0.01-1.00, Al, B, Cr, Fe, Ni 0.001-0.01. Merck Index, 8th Ed., p. 637. Pattern reviewed by K. Martin and G. McCarthy, North Dakota State University, Fargo, North Dakota, USA, \ITJCPDS Grant-in-Aid Report\RG (1990). Except for (220) reflections, there is good agreement with expermental and calculated patterns. The experimental pattern had I(220)=28; the calculated value is I(220)=49.

10 reflections in pattern.

2θ	Int.	h k l	2θ	Int.	h k l	2θ	Int.	h k l	2θ	Int.	h k l
36.9469	10	1 1 1									
42.9093	100	2 0 0									
62.3063	52	2 2 0									
74.6788	4	3 1 1									
78.6133	12	2 2 2									
93.9944	5	4 0 0									
105.6890	2	3 3 1									
109.7333	17	4 2 0									
127.1964	15	4 2 2									
143.5854	3	5 1 1									


File: MgO_lab, ID: periclase
Date: 09/25/08 14:55 Step : 0.010° Cnt Time: 0.120 Sec.
Range: 30.00 - 80.00 (Deg) Cont. Scan Rate : 5.00 Deg/min.
CPS
6475
6125
5775
5425
5075
4725
4375
4025
3675
3325
2975
2625
2275
1925
1575
1225
875
525
175
(200)
(220)
(111)
(222)
(311)
30.0
34.0
38.0
42.0
46.0
50.0
54.0
58.0
62.0
66.0
70.0
74.0
78.0
Deg.

```
*****************************************
*                                       *
* SCINTAG/USA  LATTICE REFINEMENT PROGRAM *
*                        3.00-WINNT *
*****************************************
```

CELL PARAMETERS:

A = 4.214360	B = 4.214360	C = 4.214360
ESD A = .000311	ESD B = .000311	ESD C = .000311
ALPHA = 90.000	BETA = 90.000	GAMMA = 90.000
ESD ALPHA = .000	ESD BETA = .000	ESD GAMMA = .000

VOLUME = 74.85

CRYSTAL SYMMETRY SYSTEM:

CUBIC

H	K	L	2-THETA (DEG) OBS	CALC	DELTA	Q = (1/D**2) OBS	CALC	DELTA	INT(CPS)
1	1	1	36.9053	36.9120	-.0067	.16885	.16891	-.00006	497
2	0	0	42.8687	42.8829	-.0143	.22507	.22521	-.00014	4847
2	2	0	62.2511	62.2580	-.0069	.45034	.45043	-.00009	2213
3	1	1	74.6457	74.6301	.0156	.61956	.61934	.00022	262
2	2	2	78.5663	78.5661	.0002	.67565	.67564	.00000	604

H	K	L	2-THETA (DEG) OBS	CALC	DELTA	D - SPACINGS OBS	CALC	DELTA	INT(CPS)
1	1	1	36.9053	36.9120	-.0067	2.43359	2.43316	.00042	497
2	0	0	42.8687	42.8829	-.0143	2.10785	2.10718	.00067	4847
2	2	0	62.2511	62.2580	-.0069	1.49015	1.49000	.00015	2213
3	1	1	74.6457	74.6301	.0156	1.27045	1.27068	-.00023	262
2	2	2	78.5663	78.5661	.0002	1.21658	1.21658	.00000	604

END OF LATTICE REFINEMENT

a =	0.421	nm

a =	0.421	nm
$V = a^3$	0.074618461	nm^3

Periclase MgO

Crystal Data: Cubic. *Point Group:* $4/m\ \overline{3}\ 2/m$. As small octahedra, less commonly cubo-octahedra or dodecahedra, may be clustered; granular, massive.

Physical Properties: *Cleavage:* {001}, perfect; on {111}, good; may exhibit parting on {011}. Hardness = 5.5 D(meas.) = 3.56–3.68 D(calc.) = 3.58 Slightly soluble in H_2O when powdered, to give an alkaline reaction.

Optical Properties: Transparent. *Color:* Colorless, grayish white, yellow, brownish yellow; may be green or black with inclusions; colorless in transmitted light. *Streak:* White. *Luster:* Vitreous.
Optical Class: Isotropic. $n = 1.735$–1.745

Cell Data: *Space Group:* $Fm3m$. $a = 4.203$–4.212 $Z = 4$

X-ray Powder Pattern: Synthetic.
2.106 (100), 1.489 (52), 0.9419 (17), 0.8600 (15), 1.216 (12), 2.431 (10), 1.0533 (5)

Chemistry:

	(1)
FeO	5.97
MgO	93.86
Total	99.83

(1) Monte Somma, Italy.

Mineral Group: Periclase group.

Occurrence: A product of the high-temperature metamorphism of magnesian limestones and dolostone.

Association: Forsterite, magnesite (Monte Somma, Italy); brucite, hydromagnesite, ellestadite (Crestmore quarry, California, USA); fluorellestadite, lime, periclase, magnesioferrite, hematite, srebrodolskite, anhydrite (Kopeysk, Russia).

Distribution: On Monte Somma, Campania, Italy. At Predazzo, Tirol, Austria. From Carlingford, Co. Louth, Ireland. At Broadford, Isle of Skye, and Camas Mòr, Isle of Muck, Scotland. From León, Spain. At the Bellerberg volcano, two km north of Mayen, Eifel district, Germany. From Nordmark and Långban, Värmland, Sweden. In mines around Kopeysk, Chelyabinsk coal basin, Southern Ural Mountains, Russia. In the USA, at the Crestmore quarry, Riverside Co., California; from Tombstone, Cochise Co., Arizona; in the Gabbs mine, Gabbs district, Nye Co., Nevada. In Canada, at Oka, Quebec. From ten km west of Cowell, Eyre Peninsula, South Australia.

Name: From the Greek for *to break around*, in allusion to the perfect cubic cleavage.

Type Material: Natural History Museum, Paris, France, 96.1201.

References: (1) Palache, C., H. Berman, and C. Frondel (1944) Dana's system of mineralogy, (7th edition), v. I, 499–500. (2) Deer, W.A., R.A. Howie, and J. Zussman (1962) Rock-forming minerals, v. 5, non-silicates, 1–4. (3) Hazen, R.M. (1976) Effects of temperature and pressure on the cell dimension and X-ray temperature factors of periclase. Amer. Mineral., 61, 266–271. (4) (1953) NBS Circ. 539, 1, 37.

a =	0.421	nm
$V = a^3$	0.074618461	nm^3
Density =	3.56	g/cm^3

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Density =	3.56E-21	g/nm^3
Unit Cell Mass = V x Density	2.65642E-22	g/(unit cell)

PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/

PERIOD	GROUP 1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 1.0079 **H** HYDROGEN																	2 4.0026 **He** HELIUM
2	3 6.941 **Li** LITHIUM	4 9.0122 **Be** BERYLLIUM											5 10.811 **B** BORON	6 12.011 **C** CARBON	7 14.007 **N** NITROGEN	8 15.999 **O** OXYGEN	9 18.998 **F** FLUORINE	10 20.180 **Ne** NEON
3	11 22.990 **Na** SODIUM	12 24.305 **Mg** MAGNESIUM											13 26.982 **Al** ALUMINIUM	14 28.086 **Si** SILICON	15 30.974 **P** PHOSPHORUS	16 32.065 **S** SULPHUR	17 35.453 **Cl** CHLORINE	18 39.948 **Ar** ARGON
4	19 39.098 **K** POTASSIUM	20 40.078 **Ca** CALCIUM	21 44.956 **Sc** SCANDIUM	22 47.867 **Ti** TITANIUM	23 50.942 **V** VANADIUM	24 51.996 **Cr** CHROMIUM	25 54.938 **Mn** MANGANESE	26 55.845 **Fe** IRON	27 58.933 **Co** COBALT	28 58.693 **Ni** NICKEL	29 63.546 **Cu** COPPER	30 65.39 **Zn** ZINC	31 69.723 **Ga** GALLIUM	32 72.64 **Ge** GERMANIUM	33 74.922 **As** ARSENIC	34 78.96 **Se** SELENIUM	35 79.904 **Br** BROMINE	36 83.80 **Kr** KRYPTON
5	37 85.468 **Rb** RUBIDIUM	38 87.62 **Sr** STRONTIUM	39 88.906 **Y** YTTRIUM	40 91.224 **Zr** ZIRCONIUM	41 92.906 **Nb** NIOBIUM	42 95.94 **Mo** MOLYBDENUM	43 (98) **Tc** TECHNETIUM	44 101.07 **Ru** RUTHENIUM	45 102.91 **Rh** RHODIUM	46 106.42 **Pd** PALLADIUM	47 107.87 **Ag** SILVER	48 112.41 **Cd** CADMIUM	49 114.82 **In** INDIUM	50 118.71 **Sn** TIN	51 121.76 **Sb** ANTIMONY	52 127.60 **Te** TELLURIUM	53 126.90 **I** IODINE	54 131.29 **Xe** XENON
6	55 132.91 **Cs** CAESIUM	56 137.33 **Ba** BARIUM	57-71 **La-Lu** Lanthanide	72 178.49 **Hf** HAFNIUM	73 180.95 **Ta** TANTALUM	74 183.84 **W** TUNGSTEN	75 186.21 **Re** RHENIUM	76 190.23 **Os** OSMIUM	77 192.22 **Ir** IRIDIUM	78 195.08 **Pt** PLATINUM	79 196.97 **Au** GOLD	80 200.59 **Hg** MERCURY	81 204.38 **Tl** THALLIUM	82 207.2 **Pb** LEAD	83 208.98 **Bi** BISMUTH	84 (209) **Po** POLONIUM	85 (210) **At** ASTATINE	86 (222) **Rn** RADON
7	87 (223) **Fr** FRANCIUM	88 (226) **Ra** RADIUM	89-103 **Ac-Lr** Actinide	104 (261) **Rf** RUTHERFORDIUM	105 (262) **Db** DUBNIUM	106 (266) **Sg** SEABORGIUM	107 (264) **Bh** BOHRIUM	108 (277) **Hs** HASSIUM	109 (268) **Mt** MEITNERIUM	110 (281) **Uun** UNUNNILIUM	111 (272) **Uuu** UNUNUNIUM	112 (285) **Uub** UNUNBIUM		114 (289) **Uuq** UNUNQUADIUM				

RELATIVE ATOMIC MASS (1)
GROUP IUPAC
GROUP CAS
ATOMIC NUMBER
SYMBOL
ELEMENT NAME

Metal | Semimetal | Nonmetal
1 Alkali metal
2 Alkaline earth metal
Transition metals
Lanthanide
Actinide
16 Chalcogens element
17 Halogens element
18 Noble gas

STANDARD STATE (25 °C; 101 kPa)
Ne - gas
Ga - liquid
Fe - solid
Tc - synthetic

LANTHANIDE

57 138.91 **La** LANTHANUM	58 140.12 **Ce** CERIUM	59 140.91 **Pr** PRASEODYMIUM	60 144.24 **Nd** NEODYMIUM	61 (145) **Pm** PROMETHIUM	62 150.36 **Sm** SAMARIUM	63 151.96 **Eu** EUROPIUM	64 157.25 **Gd** GADOLINIUM	65 158.93 **Tb** TERBIUM	66 162.50 **Dy** DYSPROSIUM	67 164.93 **Ho** HOLMIUM	68 167.26 **Er** ERBIUM	69 168.93 **Tm** THULIUM	70 173.04 **Yb** YTTERBIUM	71 174.97 **Lu** LUTETIUM

ACTINIDE

89 (227) **Ac** ACTINIUM	90 232.04 **Th** THORIUM	91 231.04 **Pa** PROTACTINIUM	92 238.03 **U** URANIUM	93 (237) **Np** NEPTUNIUM	94 (244) **Pu** PLUTONIUM	95 (243) **Am** AMERICIUM	96 (247) **Cm** CURIUM	97 (247) **Bk** BERKELIUM	98 (251) **Cf** CALIFORNIUM	99 (252) **Es** EINSTEINIUM	100 (257) **Fm** FERMIUM	101 (258) **Md** MENDELEVIUM	102 (259) **No** NOBELIUM	103 (262) **Lr** LAWRENCIUM

(1) Pure Appl. Chem., **73**, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@nettlinx.com)

a =	0.421	nm
$V = a^3$	0.074618461	nm^3
Density =	3.56	g/cm^3
Density =	3.56E-21	g/nm^3
Unit Cell Mass = V x Density	2.65642E-22	g/(unit cell)
Atomic Weight of Mg =	24.305	g/mole

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gfw MgO =	40.3044	g/(mole of MgO)

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gfw MgO =	40.3044	g/(mole of MgO)
(Unit Cell Mass)/(gfw MgO)	6.59089E-24	(moles of MgO)/(unit cell)

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(Unit Cell Mass)/(gfw MgO)	6.59089E-24	(moles of MgO)/(unit cell)
Avogadro's Number	6.02E+23	(formulas)/(mole of formula)

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Formulas per unit cell =	3.969690869	

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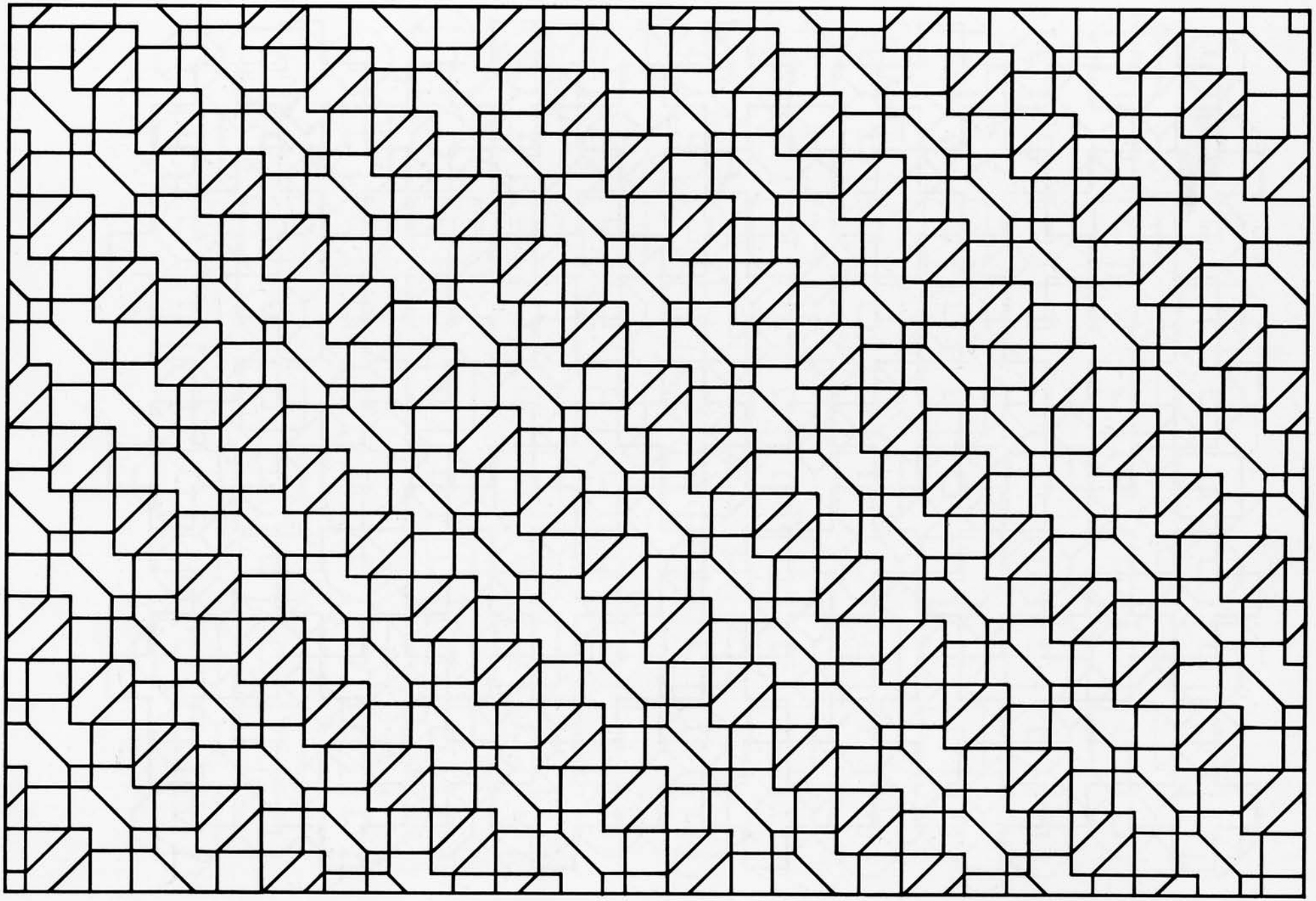
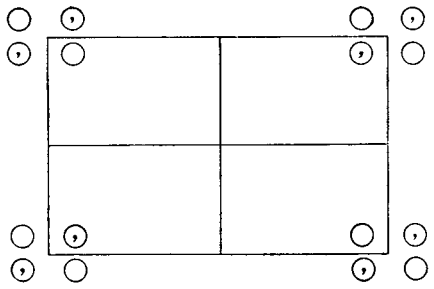
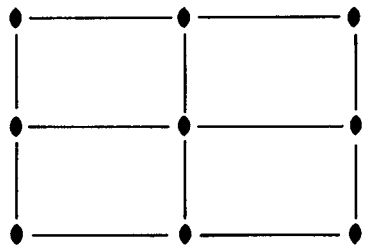
Avogadro's Number	6.02E+23	(formulas)/(mole of formula)
Formulas per unit cell =	3.969690869	
Z (must be an integer) =	4	







Origin at $2mm$

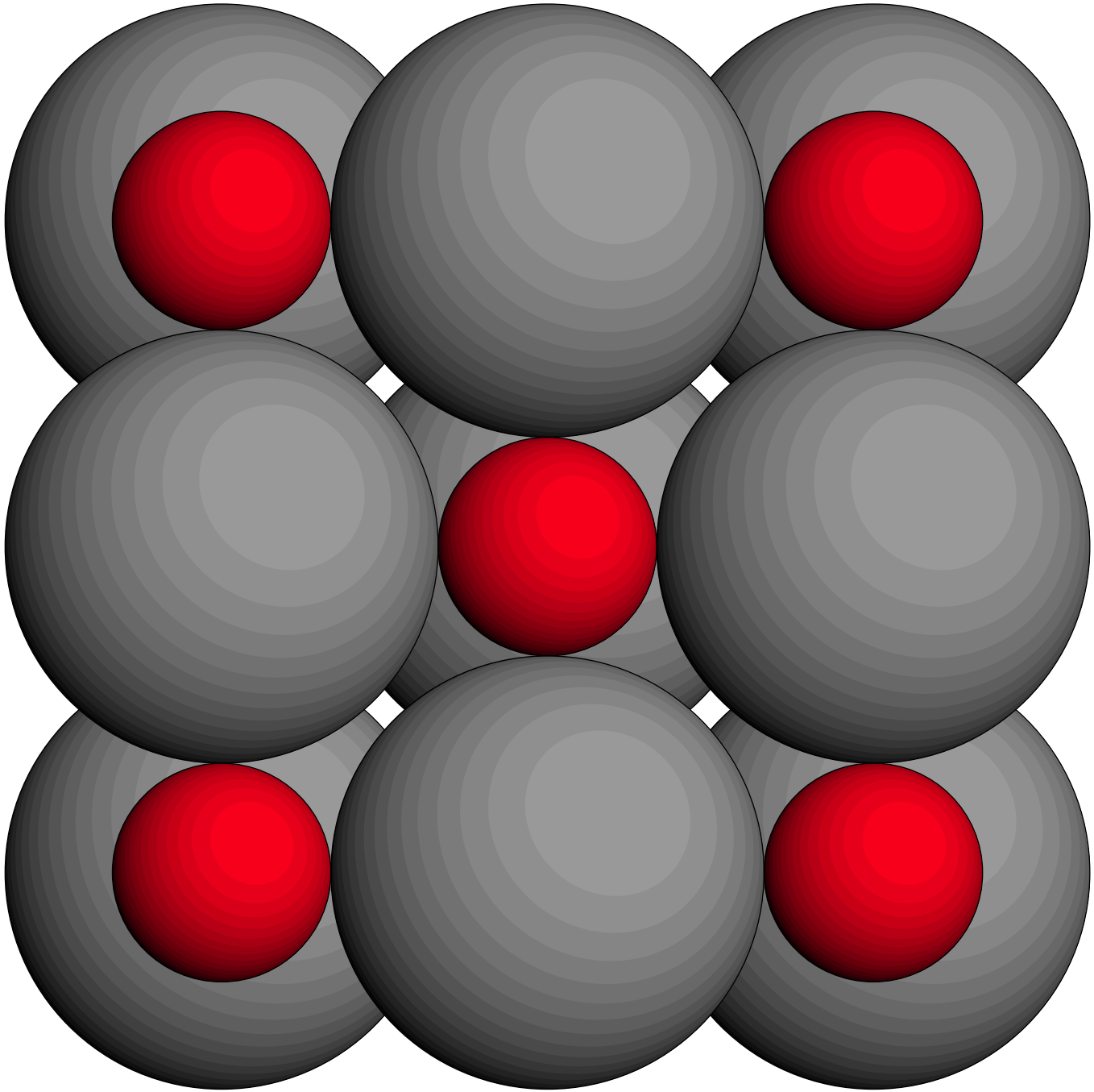
Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
				General:
4	*i*	1	x,y; $\bar{x},y$; $\bar{x},\bar{y}$; $x,\bar{y}$.	No conditions
				Special:
2	*h*	*m*	$\frac{1}{2},y$; $\frac{1}{2},\bar{y}$.	No conditions
2	*g*	*m*	$0,y$; $0,\bar{y}$.	
2	*f*	*m*	$x,\frac{1}{2}$; $\bar{x},\frac{1}{2}$.	
2	*e*	*m*	$x,0$; $\bar{x},0$.	
1	*d*	*mm*	$\frac{1}{2},\frac{1}{2}$.	
1	*c*	*mm*	$\frac{1}{2},0$.	
1	*b*	*mm*	$0,\frac{1}{2}$.	
1	*a*	*mm*	$0,0$.	

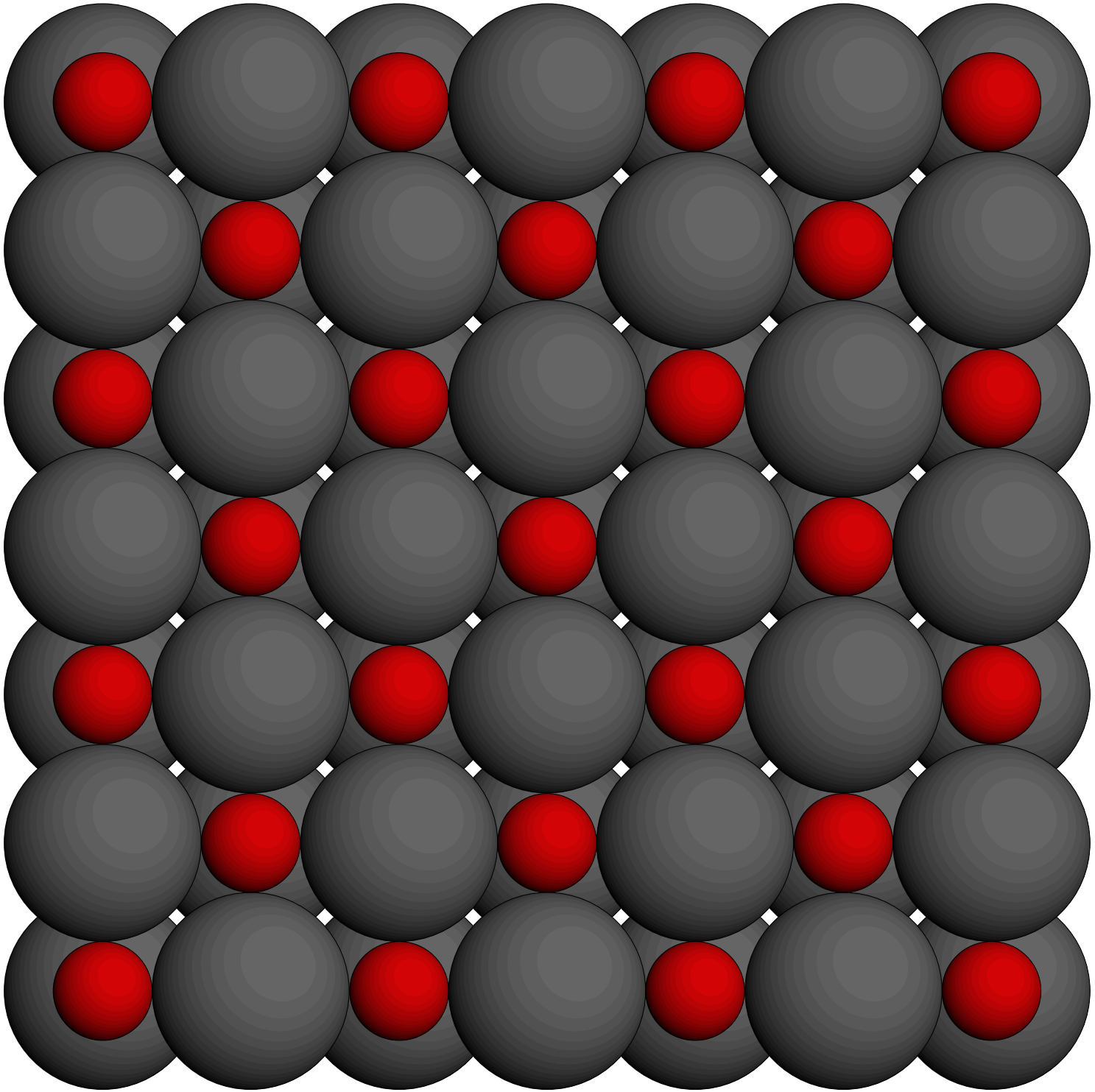
$Fm3m$ O_h^5

No. 225 $F\,4/m\,\bar{3}\,2/m$ $m\,3\,m$ Cubic

Origin at centre ($m3m$)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			$(0,0,0;\ 0,\frac{1}{2},\frac{1}{2};\ \frac{1}{2},0,\frac{1}{2};\ \frac{1}{2},\frac{1}{2},0)+$	
				General:
192	l	1	$x,y,z;\ z,x,y;\ y,z,x;\ x,z,y;\ y,x,z;\ z,y,x;$ $x,\bar{y},\bar{z};\ z,\bar{x},\bar{y};\ y,\bar{z},\bar{x};\ x,\bar{z},\bar{y};\ y,\bar{x},\bar{z};\ z,\bar{y},\bar{x};$ $\bar{x},y,\bar{z};\ \bar{z},x,\bar{y};\ \bar{y},z,\bar{x};\ \bar{x},z,\bar{y};\ \bar{y},x,\bar{z};\ \bar{z},y,\bar{x};$ $\bar{x},\bar{y},z;\ \bar{z},\bar{x},y;\ \bar{y},\bar{z},x;\ \bar{x},\bar{z},y;\ \bar{y},\bar{x},z;\ \bar{z},\bar{y},x;$ $\bar{x},\bar{y},\bar{z};\ \bar{z},\bar{x},\bar{y};\ \bar{y},\bar{z},\bar{x};\ \bar{x},\bar{z},\bar{y};\ \bar{y},\bar{x},\bar{z};\ \bar{z},\bar{y},\bar{x};$ $\bar{x},y,z;\ \bar{z},x,y;\ \bar{y},z,x;\ \bar{x},z,y;\ \bar{y},x,z;\ \bar{z},y,x;$ $x,\bar{y},z;\ z,\bar{x},y;\ y,\bar{z},x;\ x,\bar{z},y;\ y,\bar{x},z;\ z,\bar{y},x;$ $x,y,\bar{z};\ z,x,\bar{y};\ y,z,\bar{x};\ x,z,\bar{y};\ y,x,\bar{z};\ z,y,\bar{x}.$	hkl: $h+k,k+l,(l+h)=2n$ hhl: $(l+h=2n)$; C $0kl$: $(k,l=2n)$; C
				Special: as above, plus
96	k	m	$x,x,z;\ z,x,x;\ x,z,x;\ \bar{x},\bar{x},\bar{z};\ \bar{z},\bar{x},\bar{x};\ \bar{x},\bar{z},\bar{x};$ $x,\bar{x},\bar{z};\ z,\bar{x},\bar{x};\ x,\bar{z},\bar{x};\ \bar{x},x,z;\ \bar{z},x,x;\ \bar{x},z,x;$ $\bar{x},x,\bar{z};\ \bar{z},x,\bar{x};\ \bar{x},z,\bar{x};\ x,\bar{x},z;\ z,\bar{x},x;\ x,\bar{z},x;$ $\bar{x},\bar{x},z;\ \bar{z},\bar{x},x;\ \bar{x},\bar{z},x;\ x,x,\bar{z};\ z,x,\bar{x};\ x,z,\bar{x}.$	
96	j	m	$0,y,z;\ z,0,y;\ y,z,0;\ 0,z,y;\ y,0,z;\ z,y,0;$ $0,\bar{y},\bar{z};\ \bar{z},0,\bar{y};\ \bar{y},\bar{z},0;\ 0,\bar{z},\bar{y};\ \bar{y},0,\bar{z};\ \bar{z},\bar{y},0;$ $0,y,\bar{z};\ \bar{z},0,y;\ y,\bar{z},0;\ 0,\bar{z},y;\ y,0,\bar{z};\ \bar{z},y,0;$ $0,\bar{y},z;\ z,0,\bar{y};\ \bar{y},z,0;\ 0,z,\bar{y};\ \bar{y},0,z;\ z,\bar{y},0.$	no extra conditions
48	i	mm	$\frac{1}{2},x,x;\ x,\frac{1}{2},x;\ x,x,\frac{1}{2};\ \frac{1}{2},x,\bar{x};\ \bar{x},\frac{1}{2},x;\ x,\bar{x},\frac{1}{2};$ $\frac{1}{2},\bar{x},\bar{x};\ \bar{x},\frac{1}{2},\bar{x};\ \bar{x},\bar{x},\frac{1}{2};\ \frac{1}{2},\bar{x},x;\ x,\frac{1}{2},\bar{x};\ \bar{x},x,\frac{1}{2}.$	
48	h	mm	$0,x,x;\ x,0,x;\ x,x,0;\ 0,x,\bar{x};\ \bar{x},0,x;\ x,\bar{x},0;$ $0,\bar{x},\bar{x};\ \bar{x},0,\bar{x};\ \bar{x},\bar{x},0;\ 0,\bar{x},x;\ x,0,\bar{x};\ \bar{x},x,0.$	
48	g	mm	$x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},x;\ x,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},x,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},x;$ $\bar{x},\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\bar{x};\ \bar{x},\frac{1}{4},\frac{3}{4};\ \frac{3}{4},\bar{x},\frac{1}{4};\ \frac{1}{4},\frac{3}{4},\bar{x}.$	hkl: $h,(k,l)=2n$
32	f	$3m$	$x,x,x;\ x,\bar{x},\bar{x};\ \bar{x},x,\bar{x};\ \bar{x},\bar{x},x;$ $\bar{x},\bar{x},\bar{x};\ \bar{x},x,x;\ x,\bar{x},x;\ x,x,\bar{x}.$	no extra conditions
24	e	$4mm$	$x,0,0;\ 0,x,0;\ 0,0,x;\ \bar{x},0,0;\ 0,\bar{x},0;\ 0,0,\bar{x}.$	
24	d	mmm	$0,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},0;\ 0,\frac{1}{4},\frac{3}{4};\ \frac{3}{4},0,\frac{1}{4};\ \frac{1}{4},\frac{3}{4},0.$	hkl: $h,(k,l)=2n$
8	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4};\ \frac{3}{4},\frac{3}{4},\frac{3}{4}.$	
4	b	$m3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}.$	no extra conditions
4	a	$m3m$	$0,0,0.$	





Lecture Notes - Mineralogy - Periclase Structure

- In lab we determined the unit cell for a crystal of synthetic periclase (MgO). Because periclase is cubic, only one lattice parameter (**a**) is needed to completely specify the size and shape of the unit cell. We found that **a** = 0.421 nm (= 4.21 Å). Based on this measurement, the volume (**V**) of the periclase unit cell is 0.074618 nm^3.

- The density of periclase can be determined by a specific gravity measurement using either the Joly or Berman balance. Because periclase is very hygroscopic, the Berman balance with toluene as the fluid is to be recommended. Periclase has a density of 3.56 g/cm^3 (=3.56 x 10^{-21} g/nm^3). One unit cell contains 2.6564 x 10^{-22} gm of periclase. [(0.074618 nm^3/unit cell) x (3.56 x 10^{-21} gm of periclase/nm^3) = (2.6564 x 10^{-22} gm of periclase/unit cell)]

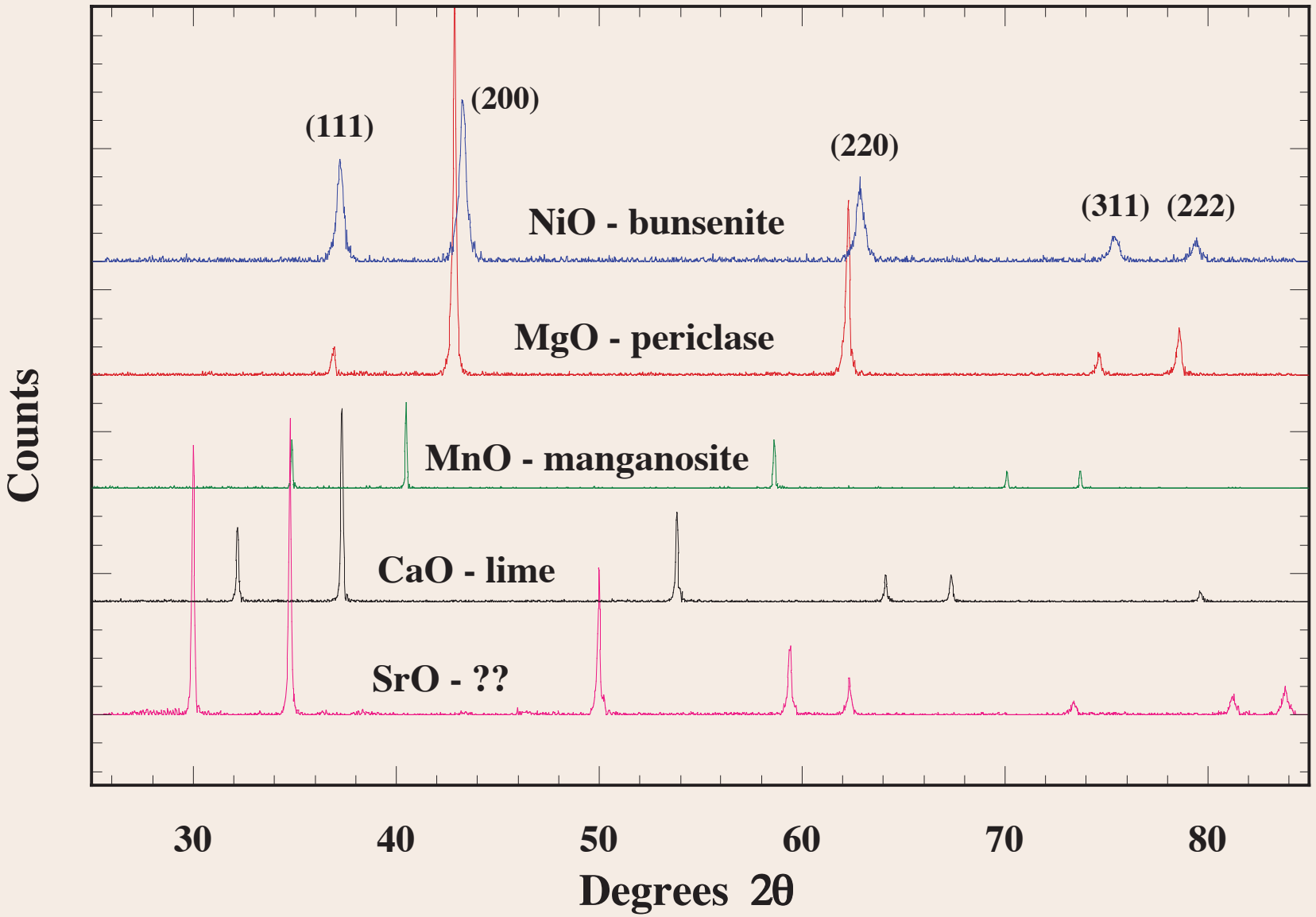
- One gram formula unit (mole) of periclase has a mass (**gfw**) of 40.31 gms and contains **N** (6.023 x 10^{23}) formula units of MgO. Therefore, there are [(6.023 x 10^{23} formula units of MgO)/(40.31 gms) =] 1.494 x 10^{22} formula units of periclase per gram of periclase.

- Using the results of (2) and (3) it is clear that there should be [(1.494 x 10^{22} formula units of periclase/gm of periclase) x (2.6564 x 10^{-22} gm of periclase/unit cell) =] 3.969 formula units of periclase/unit cell. This number **Z** (formula units/unit cell) must be an integer (**Z** = 4) because there cannot be fractions of atoms in the unit cell.

$$\mathbf{Z}\left(\frac{\text{formula units}}{\text{unit cell}}\right) = \frac{\mathbf{V\,D\,N}}{\mathbf{M}} \; \frac{\left(\frac{\text{nm}^3}{\text{unit cell}}\right)\left(\frac{\text{gm}}{\text{cm}^3}\right)\left(\frac{\text{formula units}}{\text{mole}}\right)}{\left(\frac{\text{gm}}{\text{mole}}\right)}$$

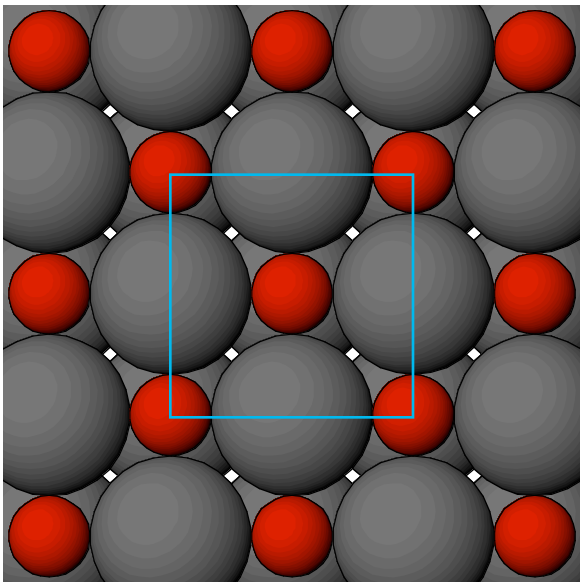
- Knowing the value of **Z**, it is possible to determine the exact locations of the Mg and O atoms using the special positions for the periclase space group Fm3m. With the multiplicity of a general position equal to 192, it is clear that Mg and O must be on special positions indeed. From the *International Tables for X-ray Crystallography* (p.338), it is clear that Mg and O **must** occupy special positions *a* and *b* with coordinates 0,0,0 and $^1/_2,^1/_2,^1/_2$, respectively. But which atom is to have 0,0,0 and which is to have $^1/_2,^1/_2,^1/_2$? Careful scrutiny of the structure reveals that there is no difference between the two possibilities; there is only a difference in choice of origin.

- Other crystal structures may be discovered in the same manner as that of periclase. However, for structures with more complexity, data in addition to Z and the crystal's symmetry are required for a complete structure determination.


(111)
(200)
(220)
(311)
(222)
NiO - bunsenite
MgO - periclase
MnO - manganosite
CaO - lime
SrO - ??
Counts
30
40
50
60
70
80
Degrees 2θ

Mineralogy Lab
Measuring Atoms

X-ray diffraction may be used to measure the spacing between planes of atoms in a crystal. The figure is a model of the crystal structure of the isometric mineral periclase (MgO) viewed down the c-axis (a-axis points down the page, b-axis points right). The end of a face-centered unit cell is shown in blue. Mg atoms are shown in red and O atoms are shown in gray. The spacing of the horizontal rows of red atoms represent the spacing of the atoms that produce the (002) x-ray peak. The spacing of the (001) peak (never observed) is given by the unit cell edge. $d_{(001)} = 2 \times d_{(002)}$.



All of the following list of minerals has a simple oxide with a crystal structure like periclase:

(a) bunsenite (NiO)
(b) lime (CaO)
(c) manganosite (MnO)
(d) periclase (MgO)
(e) unnamedite (SrO)

These minerals are isostructural with each other. A powder diffraction pattern is shown for each on the attached pages. These patterns were collected using the Smith diffractometer, which has a Cu x-ray tube (CuKα = 0.1540 nm).

(1) With your lab group, collect a diffraction pattern for one of these oxides. Scan from 25-85° (2θ) at 5° per minute. Identify the peaks by comparing your pattern with the PDF data file. Print out your pattern with the peaks labeled.

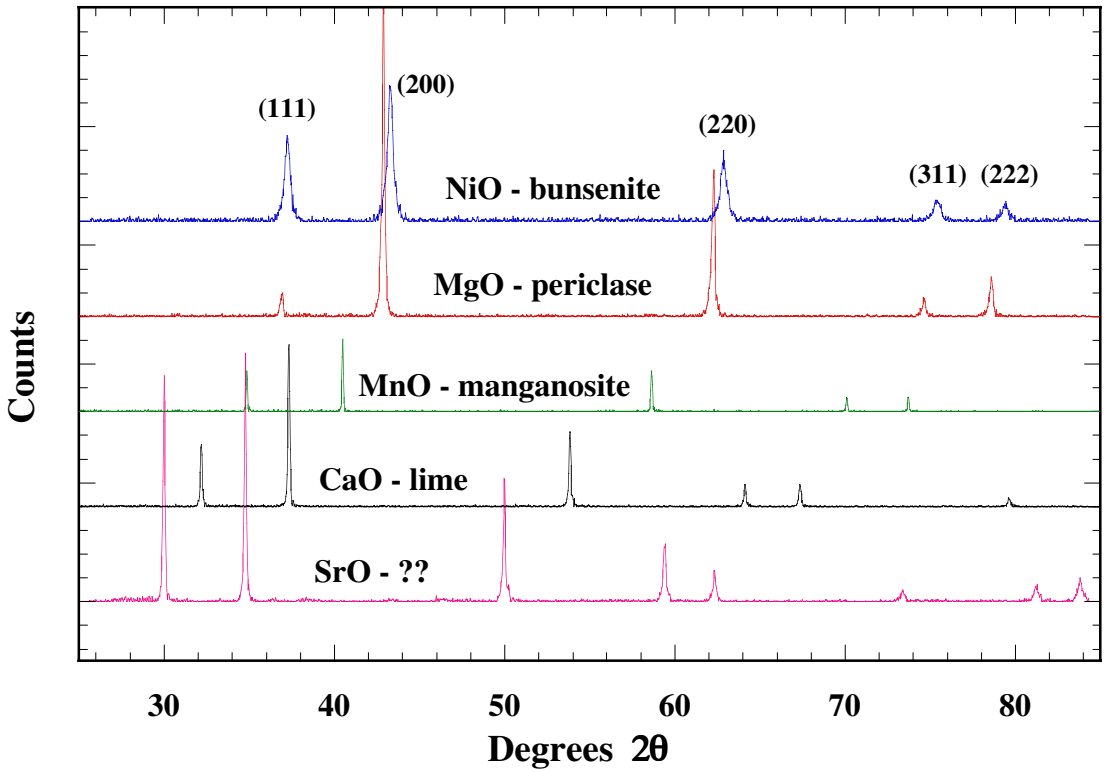
(2) Use the Scintag crystallography software to determine the one unit cell parameter (**a**).

(3) Using the (002) peak from your pattern, calculate the size of the unit cell using Bragg's Law.

(4) Assuming that the radius of the oxygen atoms is 0.140 nm, calculate the size of the metal atom in your mineral. Give an uncertainty for your answer.

(5) Is your answer reasonable? How does it compare with the radius given in the book?

Figure 1.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NiO - bunsenite
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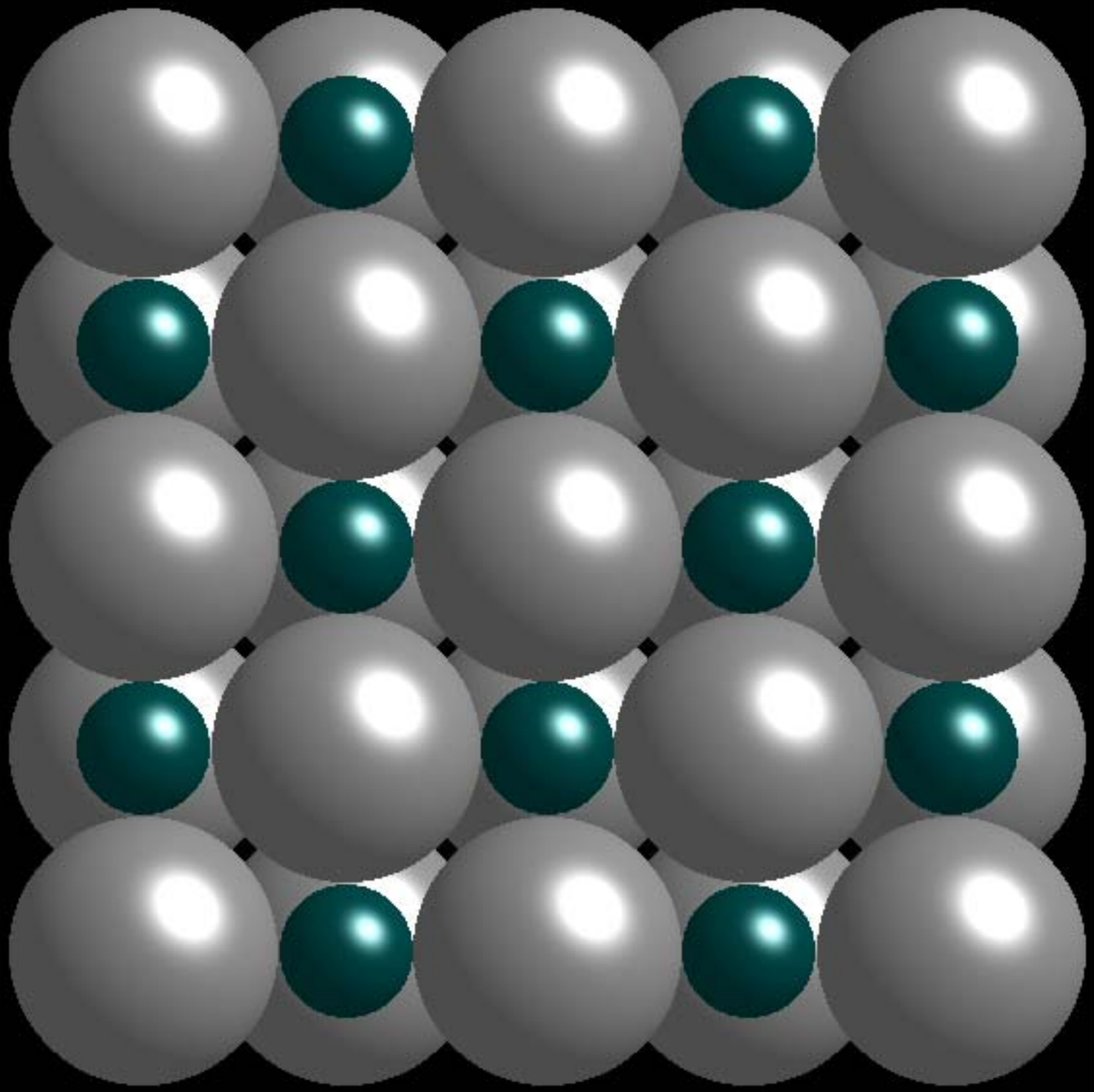
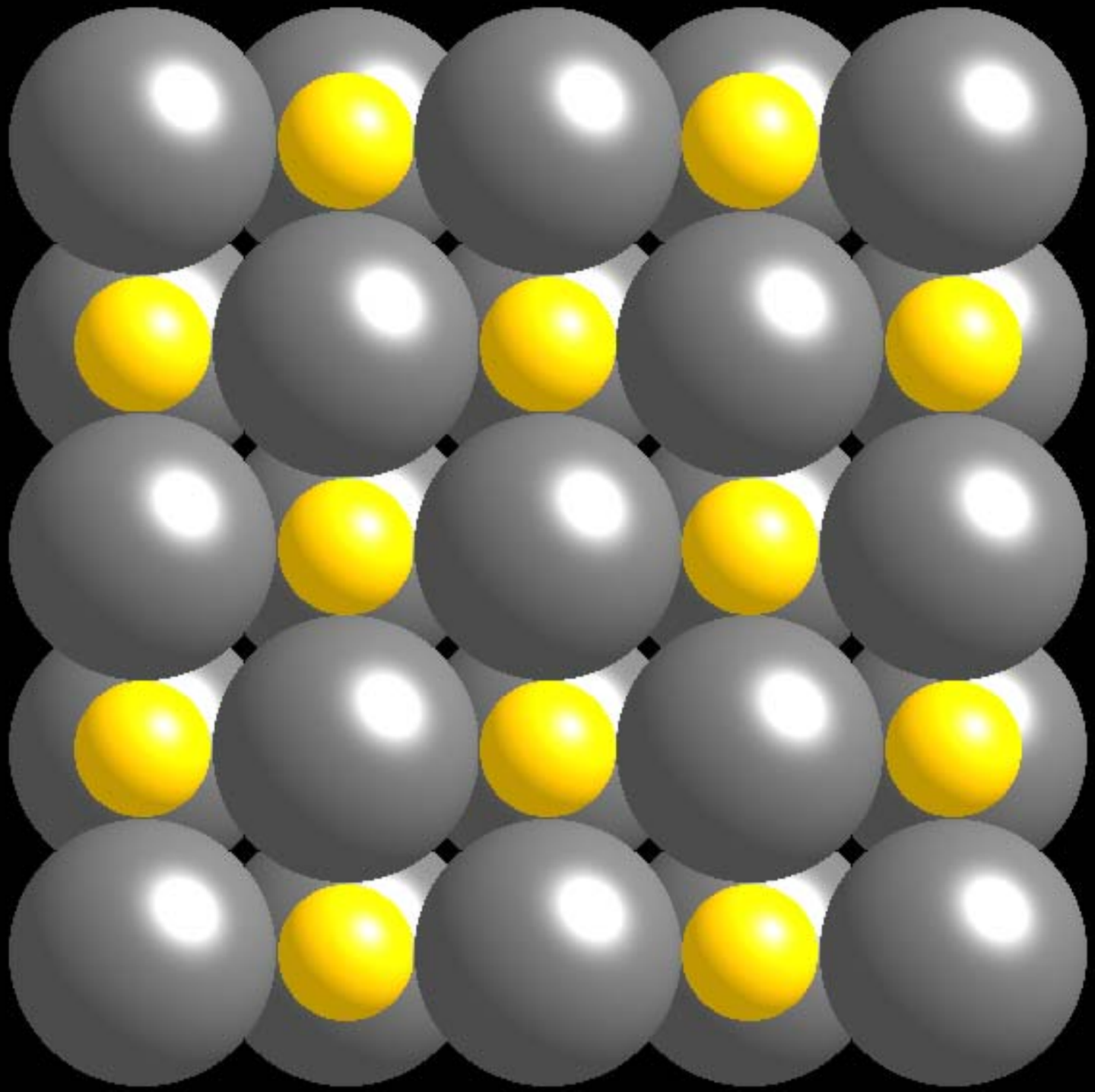
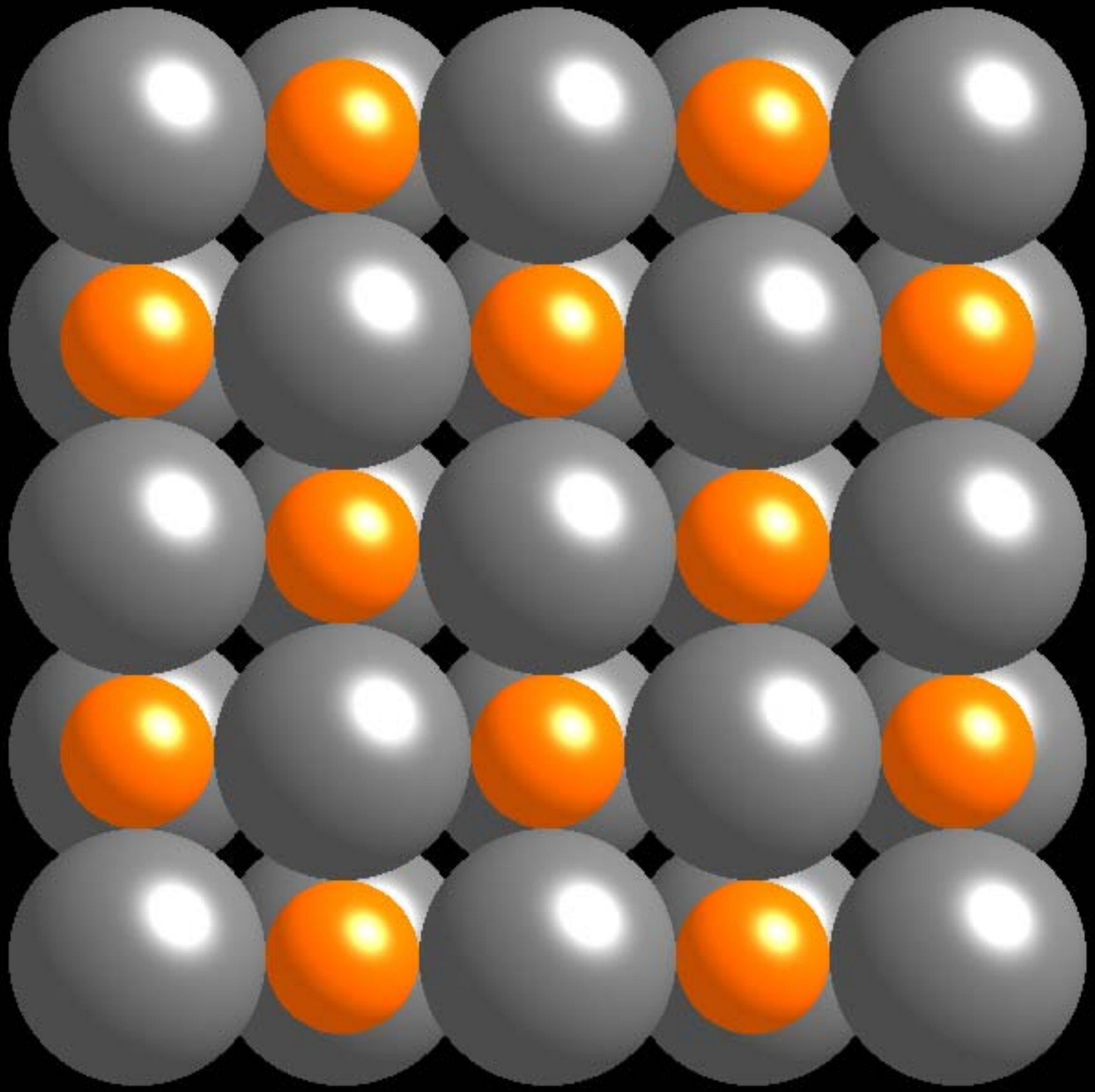
Degrees 2θ



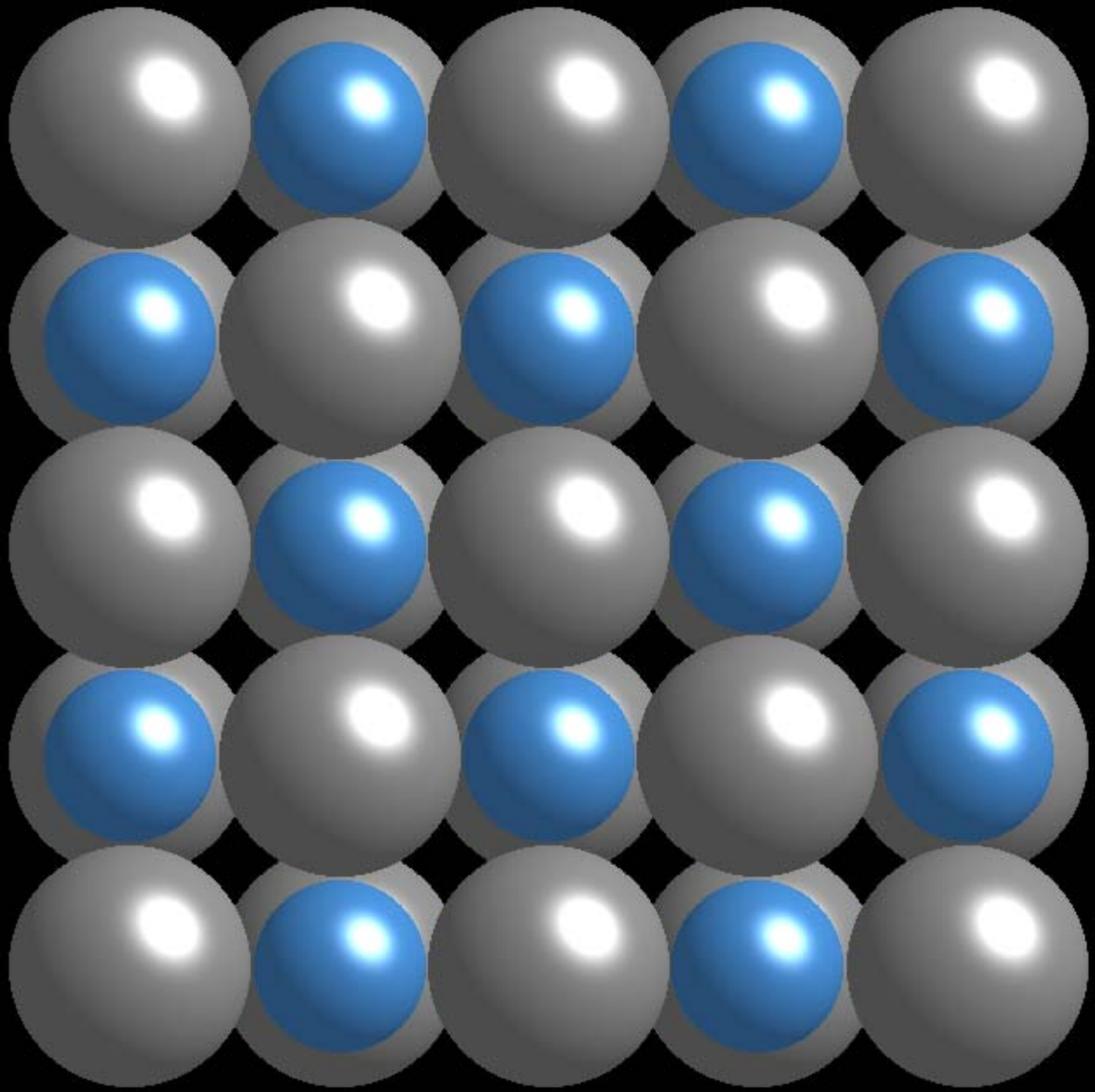
NiO



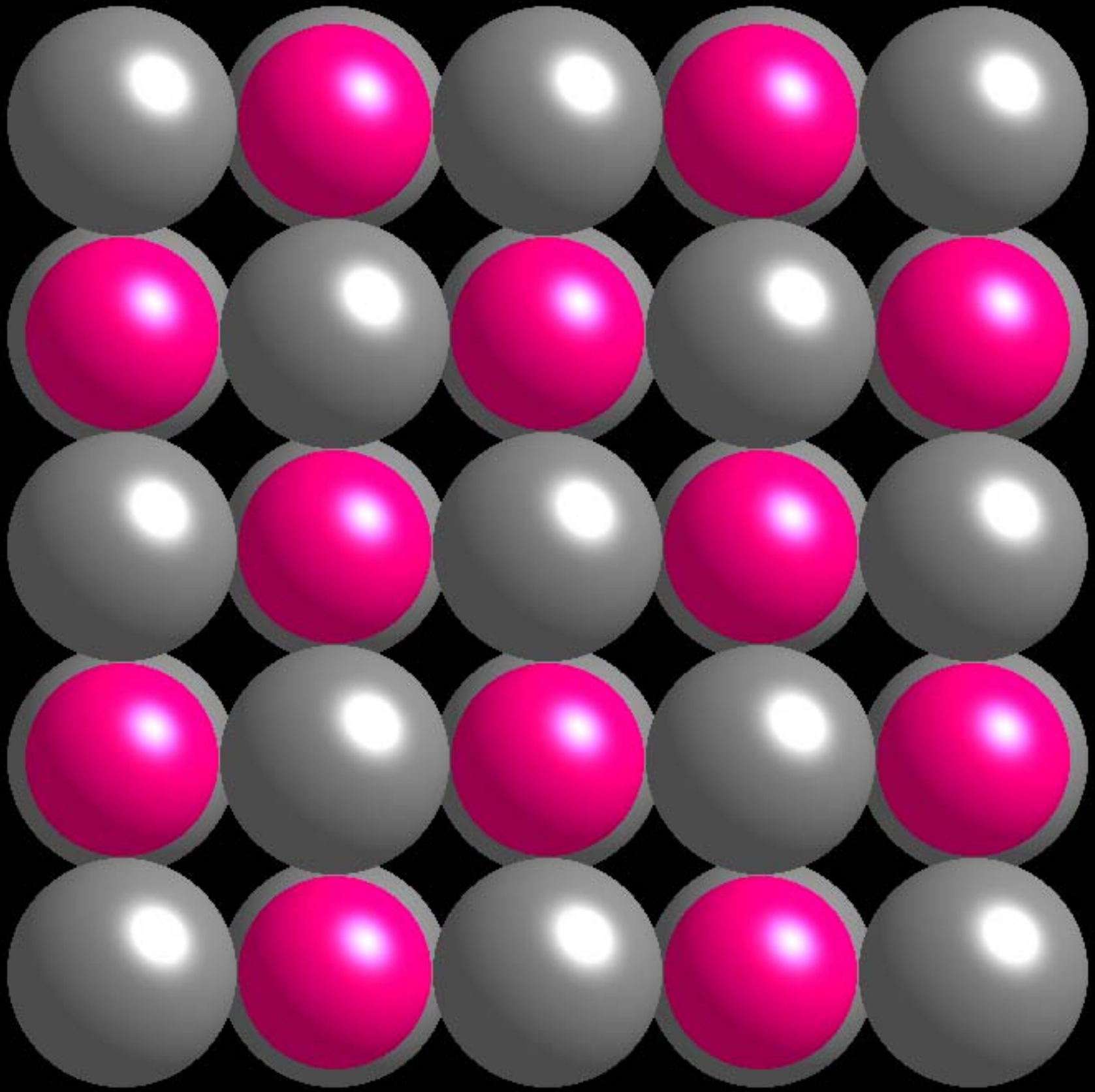
MgO



MnO



CaO


SrO