

# Unpacking the crystal structure



x-ray powder diffraction



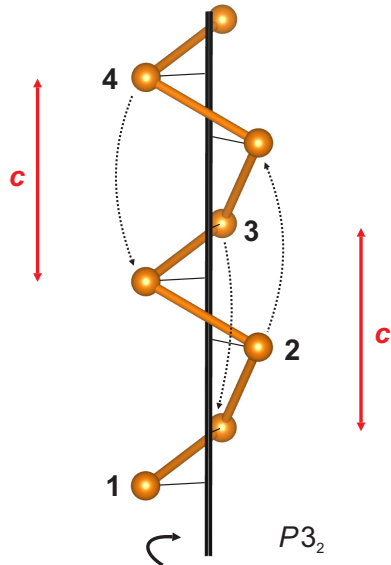
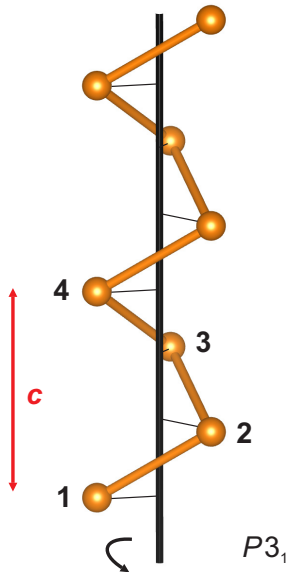
diamond



William Bragg



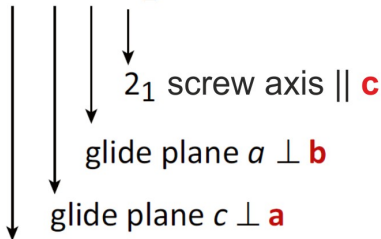
# Helical chains in tellurium



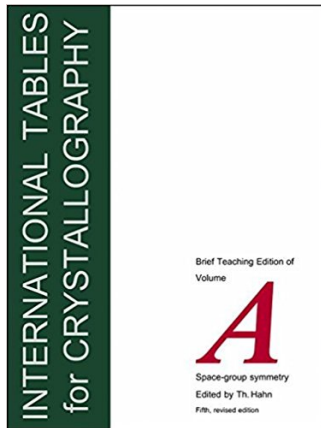
"Generators"

*symmetry elements with respect to three given viewing directions*

$P c a 2_1$  (orthorhombic)



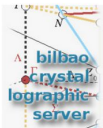
Bravais type  
(kind of centering)



Space groups and symmetries = **vol. A**



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In forthcoming schools and workshops

### News:

- **New Article in Nature**  
10/2020: Xu *et al.* "High-throughput calculations of magnetic topological materials" *Nature* (2020) **586**, 702-707.
- New programs:  
**MRANDREP**

### Space-group symmetry

<a href="#">GENPOS</a>	Generators and General Positions of Space Groups
<a href="#">WYCKPOS</a>	Wyckoff Positions of Space Groups
<a href="#">HKLCOND</a>	Reflection conditions of Space Groups
<a href="#">MAXSUB</a>	Maximal Subgroups of Space Groups
<a href="#">SERIES</a>	Series of Maximal Isomorphic Subgroups of Space Groups
<a href="#">WYCKSETS</a>	Equivalent Sets of Wyckoff Positions
<a href="#">NORMALIZER</a>	Normalizers of Space Groups
<a href="#">KVEC</a>	The k-vector types and Brillouin zones of Space Groups
<a href="#">SYMMETRY OPERATIONS</a>	Geometric interpretation of matrix column representations of symmetry operations
<a href="#">IDENTIFY GROUP</a>	Identification of a Space Group from a set of generators in an arbitrary setting

### Magnetic Symmetry and Applications

Quick access to some tables

Space Groups

Plane Groups

Layer Groups

Rod Groups

Frieze Groups

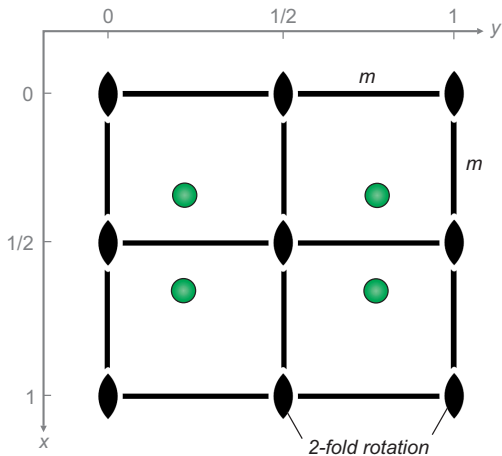
2D Point Groups

Lists of space groups, Wyckoff positions:

<http://cryst.ehu.es>

# Each space groups has a number!

1	$P1$	2	$P-1$	3	$P2$	4	$P2_1$	5	$C2$
6	$Pm$	7	$Pc$	8	$Cm$	9	$Cc$	10	$P2/m$
11	$P2_1/m$	12	$C2/m$	13	$P2/c$	14	$P2_1/c$	15	$C2/c$
16	$P222$	17	$P222_1$	18	$P2_12_12$	19	$P2_12_12_1$	20	$C222_1$
21	$C222$	22	$F222$	23	$I222$	24	$I2_12_12_1$	25	$Pmm2$
26	$Pmc2_1$	27	$Pcc2$	28	$Pma2$	29	$Pca2_1$	30	$Pnc2$
31	$Pmn2_1$	32	$Pba2$	33	$Pna2_1$	34	$Pnn2$	35	$Cmm2$
36	$Cmc2_1$	37	$Ccc2$	38	$Amm2$	39	$Aem2$	40	$Ama2$
41	$Aea2$	42	$Fmm2$	43	$Fdd2$	44	$Imm2$	45	$Iba2$
46	$Ima2$	47	$Pmmm$	48	$Pnnn$	49	$Pccm$	50	$Pban$
51	$Pmma$	52	$Pnna$	53	$Pmna$	54	$Pcca$	55	$Pbam$
56	$Pccn$	57	$Pbcm$	58	$Pnnm$	59	$Pmnm$	60	$Pbcn$
61	$Pbca$	62	$Pnma$	63	$Cmcm$	64	$Cmce$	65	$Cmmm$

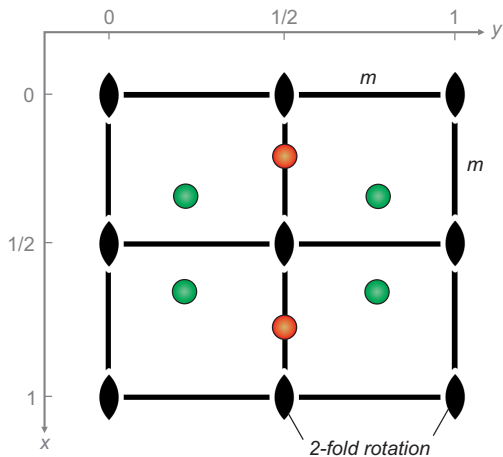


### Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4	<i>i</i>	1	(1) $x, y, z$ (3) $x, \bar{y}, z$	(2) $\bar{x}, \bar{y}, z$ (4) $\bar{x}, y, z$
2	<i>h</i>	$m \dots$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$
2	<i>g</i>	$m \dots$	$0, y, z$	$0, \bar{y}, z$
2	<i>f</i>	$\dots m$	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$
2	<i>e</i>	$\dots m$	$x, 0, z$	$\bar{x}, 0, z$
1	<i>d</i>	$m m 2$	$\frac{1}{2}, \frac{1}{2}, z$	
1	<i>c</i>	$m m 2$	$\frac{1}{2}, 0, z$	
1	<i>b</i>	$m m 2$	$0, \frac{1}{2}, z$	
1	<i>a</i>	$m m 2$	$0, 0, z$	



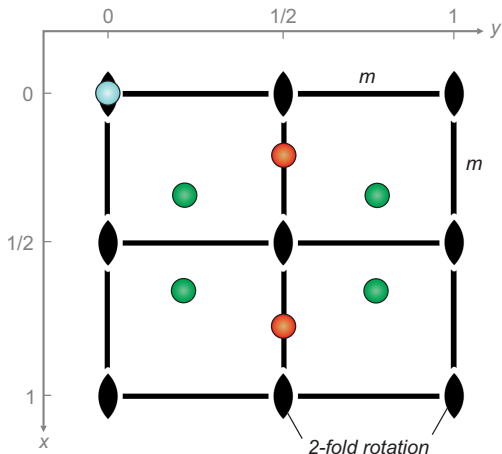
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2	<i>h</i>	$m \dots$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$
2	<i>g</i>	$m \dots$	$0, y, z$	$0, \bar{y}, z$
2	<i>f</i>	$\dots m$	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$
2	<i>e</i>	$\dots m$	$x, 0, z$	$\bar{x}, 0, z$
1	<i>d</i>	$mm2$	$\frac{1}{2}, \frac{1}{2}, z$	
1	<i>c</i>	$mm2$	$\frac{1}{2}, 0, z$	
1	<i>b</i>	$mm2$	$0, \frac{1}{2}, z$	
1	<i>a</i>	$mm2$	$0, 0, z$	





## Positions

Multiplicity,  
Wyckoff letter,  
Site symmetry

Coordinates

4	<i>i</i>	1	(1) $x, y, z$ (3) $x, \bar{y}, z$	(2) $\bar{x}, \bar{y}, z$ (4) $\bar{x}, y, z$
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2	<i>h</i>	$m \dots$	$\frac{1}{2}, y, z$	$\frac{1}{2}, \bar{y}, z$
---	----------	-----------	---------------------	---------------------------

2	<i>g</i>	$m \dots$	$0, y, z$	$0, \bar{y}, z$
---	----------	-----------	-----------	-----------------

2	<i>f</i>	$\dots m$	$x, \frac{1}{2}, z$	$\bar{x}, \frac{1}{2}, z$
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2	<i>e</i>	$\dots m$	$x, 0, z$	$\bar{x}, 0, z$
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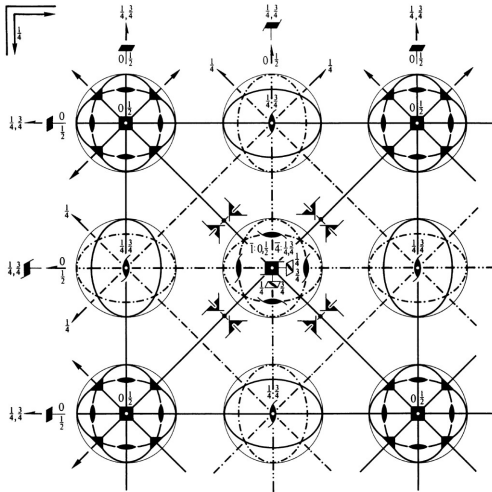
1	<i>d</i>	$mm2$	$\frac{1}{2}, \frac{1}{2}, z$	
---	----------	-------	-------------------------------	--

1	<i>c</i>	$mm2$	$\frac{1}{2}, 0, z$	
---	----------	-------	---------------------	--

1	<i>b</i>	$mm2$	$0, \frac{1}{2}, z$	
---	----------	-------	---------------------	--

1	<i>a</i>	$mm2$	$0, 0, z$	
---	----------	-------	-----------	--

# Things may grow complicated...



$Fm\bar{3}m$

No. 225

$O_h^5$

$F 4/m \bar{3} 2/m$

192 1 1

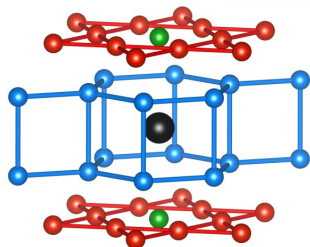
- |                                  |                                  |                                  |                                  |
|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| (1) $x, y, z$                    | (2) $\bar{x}, \bar{y}, z$        | (3) $\bar{x}, y, \bar{z}$        | (4) $x, \bar{y}, \bar{z}$        |
| (5) $z, x, y$                    | (6) $z, \bar{x}, \bar{y}$        | (7) $\bar{z}, \bar{x}, y$        | (8) $\bar{z}, x, \bar{y}$        |
| (9) $y, z, x$                    | (10) $\bar{y}, z, \bar{x}$       | (11) $y, \bar{z}, \bar{x}$       | (12) $\bar{y}, \bar{z}, x$       |
| (13) $y, x, \bar{z}$             | (14) $\bar{y}, \bar{x}, \bar{z}$ | (15) $y, \bar{x}, z$             | (16) $\bar{y}, x, z$             |
| (17) $x, z, \bar{y}$             | (18) $\bar{x}, z, y$             | (19) $\bar{x}, \bar{z}, \bar{y}$ | (20) $x, \bar{z}, y$             |
| (21) $z, y, \bar{x}$             | (22) $z, \bar{y}, x$             | (23) $\bar{z}, y, x$             | (24) $\bar{z}, \bar{y}, \bar{x}$ |
| (25) $\bar{x}, \bar{y}, \bar{z}$ | (26) $x, y, \bar{z}$             | (27) $x, \bar{y}, z$             | (28) $\bar{x}, y, z$             |
| (29) $\bar{z}, \bar{x}, \bar{y}$ | (30) $\bar{z}, x, y$             | (31) $z, x, \bar{y}$             | (32) $z, \bar{x}, y$             |
| (33) $\bar{y}, \bar{z}, \bar{x}$ | (34) $y, \bar{z}, x$             | (35) $\bar{y}, z, x$             | (36) $y, z, \bar{x}$             |
| (37) $\bar{y}, \bar{x}, z$       | (38) $y, x, z$                   | (39) $\bar{y}, x, \bar{z}$       | (40) $y, \bar{x}, \bar{z}$       |
| (41) $\bar{x}, \bar{z}, y$       | (42) $x, \bar{z}, \bar{y}$       | (43) $x, z, y$                   | (44) $\bar{x}, z, \bar{y}$       |
| (45) $\bar{z}, \bar{y}, x$       | (46) $\bar{z}, y, \bar{x}$       | (47) $z, \bar{y}, \bar{x}$       | (48) $z, y, x$                   |

$$a = b = 5.4651(2) \text{ \AA}, \quad c = 8.637(7) \text{ \AA}$$

$$V = 223.4(2) \text{ \AA}^3$$

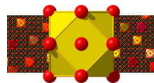
$$P6/mmm$$

Atom	$x/a$	$y/b$	$z/c$
Cs	0	0	0
V	0.5	0.5	0.5
Sb1	0	0	0.5
Sb2	$\frac{2}{3}$	$\frac{1}{3}$	0.7591(11)



Composition: **CsV<sub>3</sub>Sb<sub>5</sub>**, but only Wyckoff positions are listed:  
Cs (1a), V (3g), Sb1 (1b), Sb2 (4h)

- Open Crystallography Database (COD)  
all types of compounds (493 620 entries), **free**
- Inorganic Crystal Structure Database (ICSD)  
“Karlsruhe database” (260 000 entries), **commercial**  
(Uni Leipzig has access)
- Cambridge Structural Database (CSD)  
mostly organic compounds (1.1 million entries), **commercial**
- Pearson's Crystal Data  
inorganic and especially intermetallic compounds  
(380 000 entries), **commercial**



```

_cell_length_a      3.0823
_cell_length_b      3.0823
_cell_length_c      3.51461
_cell_angle_alpha   90
_cell_angle_beta    90
_cell_angle_gamma   120

```

**Lattice  
parameters**  
in units of Å

```

_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
Mg1 Mg 0 0 0
B1 B 0.3333 0.6667 0.5

```

**Atomic positions**  
*fractional coordinates*

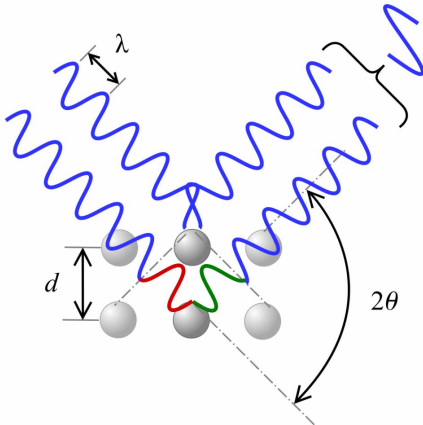
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_symmetry_space_group_name_Hall '-P 6 2'
_symmetry_space_group_name_H-M 'P 6/m m m'

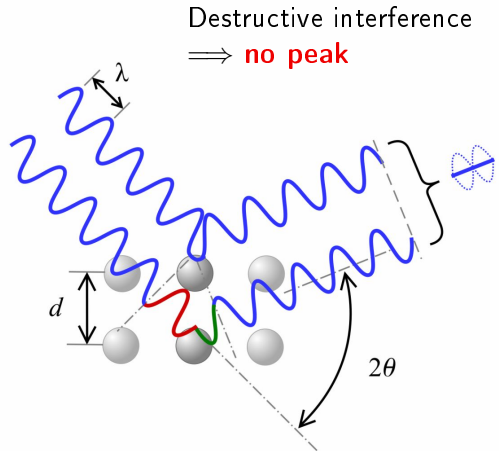
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**Symmetry**

$$2d \sin \theta = n\lambda$$



Constructive interference  
 $\Rightarrow$  **Bragg peak**

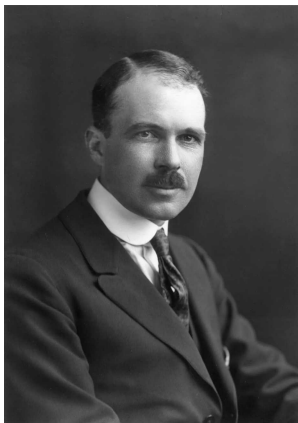


Destructive interference  
 $\Rightarrow$  **no peak**



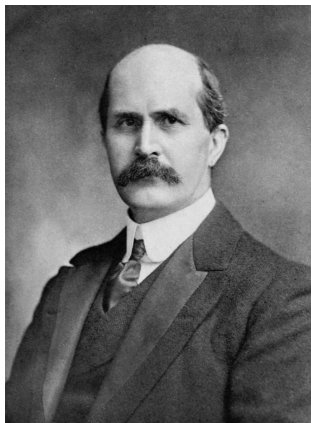
Person

*William Bragg*



William Lawrence Bragg  
1890–1971

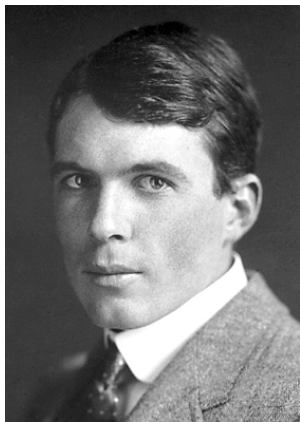
*Son*



William Henry Bragg  
1862–1942

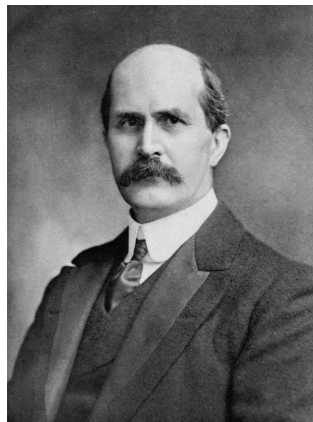
*Father*





William Lawrence Bragg  
1890–1971

*Son*

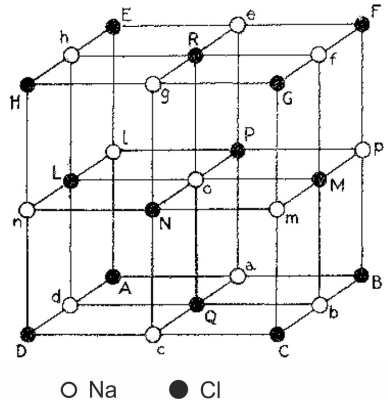


William Henry Bragg  
1862–1942

*Father*

**Nobel prize (1915)**

# Braggs' common spectrometer



NaCl: the first crystal structure resolved experimentally

# Braggs' common spectrometer

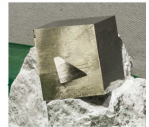
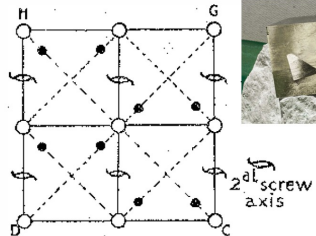
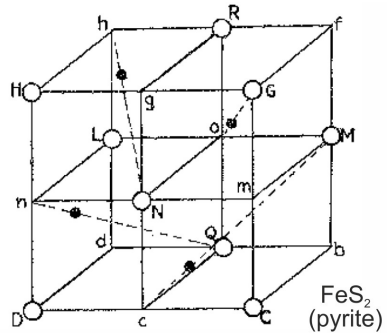
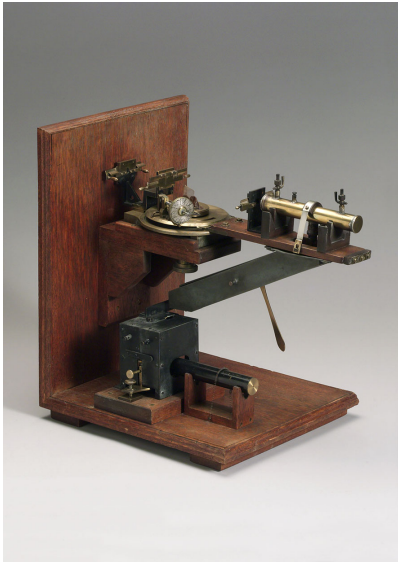


Image credits: Science Museum London (CC-BY-SA), Proc. Royal Soc. London 89, 468 (1914), Raimond Spekking (CC-BY-SA)



# Experimental technique

*x-ray diffraction*

# X-ray powder diffractometer

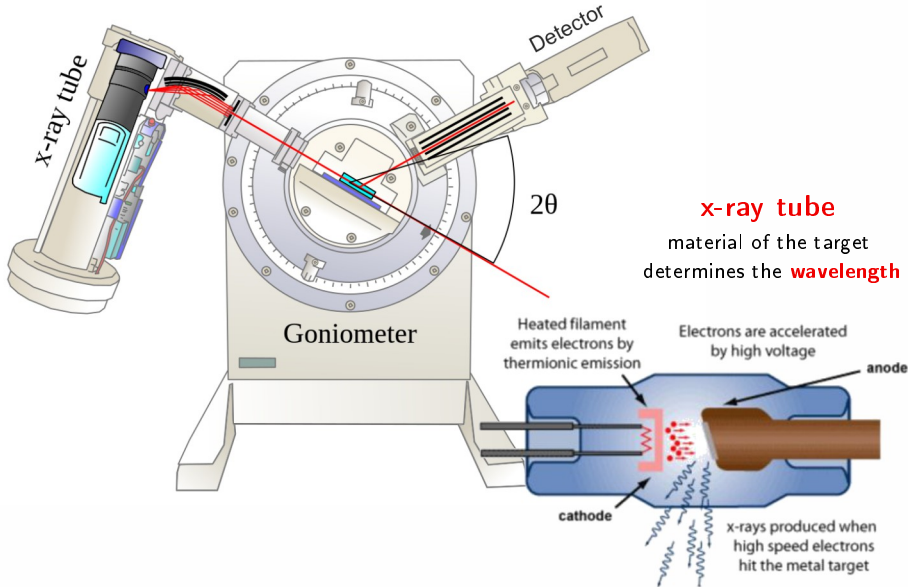
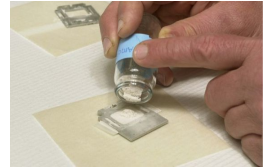
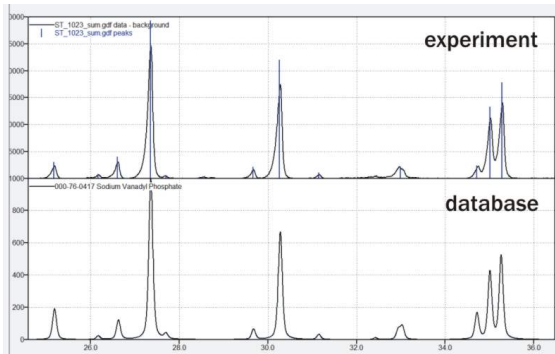
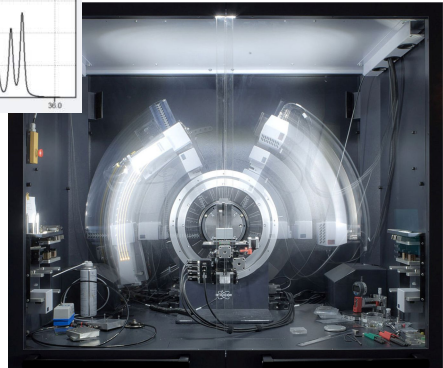
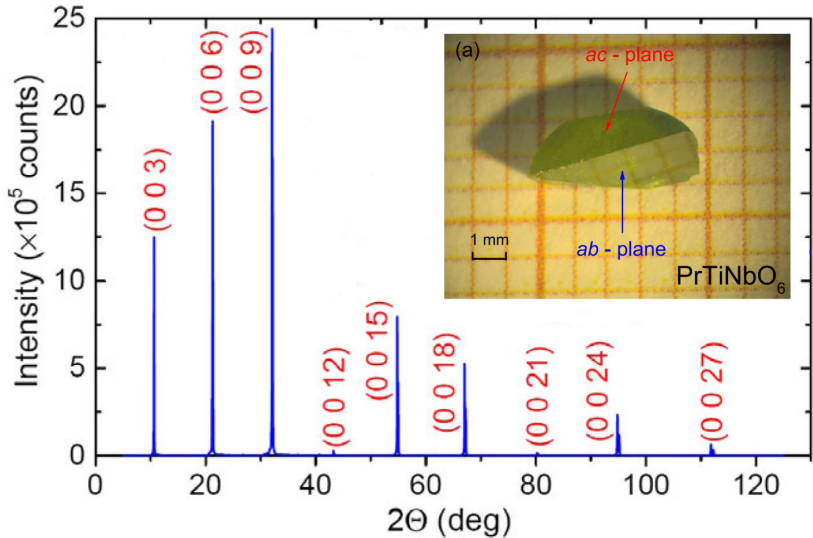


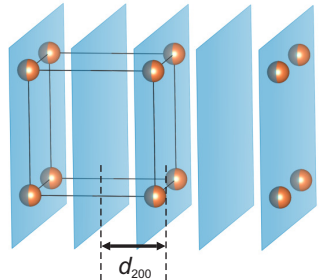
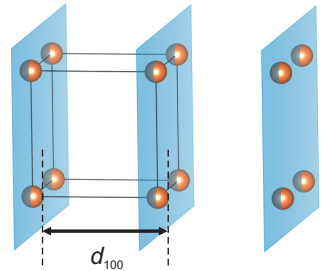
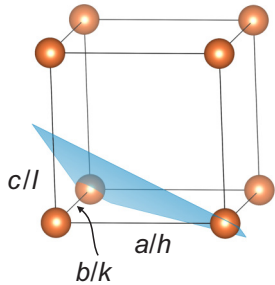
Image credits: LibreText Chemistry and Free Mineralogy Textbook (CC-BY-SA)



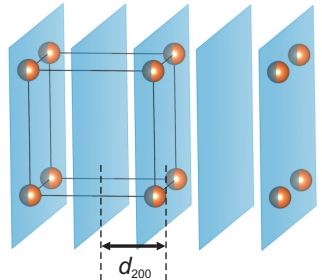
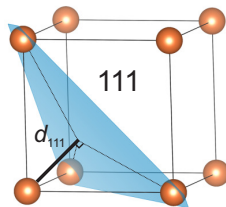
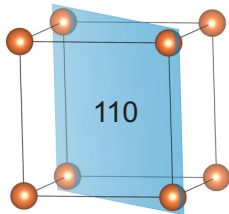
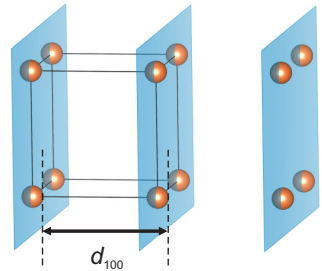
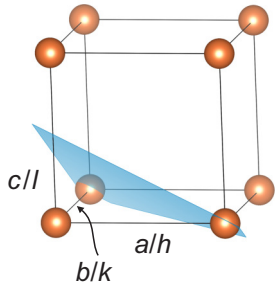
XRD pattern serves  
as a **fingerprint**  
of the chemical compound











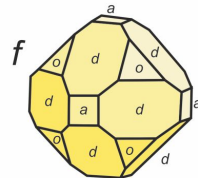
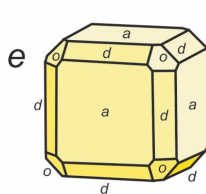
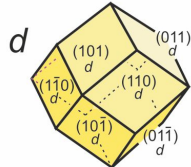
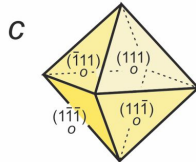
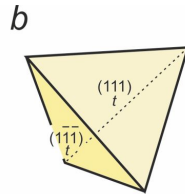
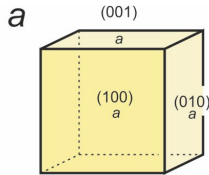
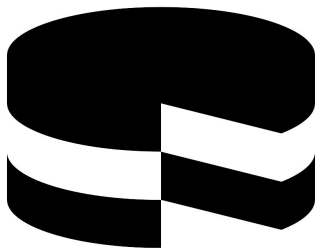


Image credits: Free Mineralogy Textbook, Robert Lavinsky, Parent Géry, and Juan Buelga (CC-BY-SA)



Material

*diamond*

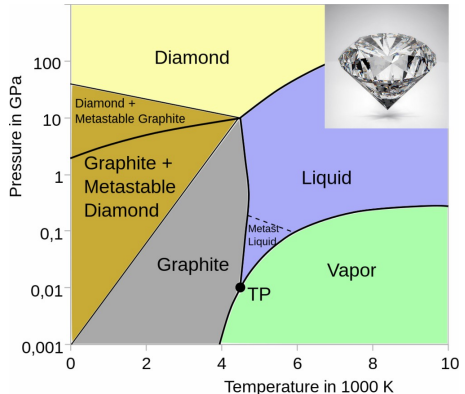


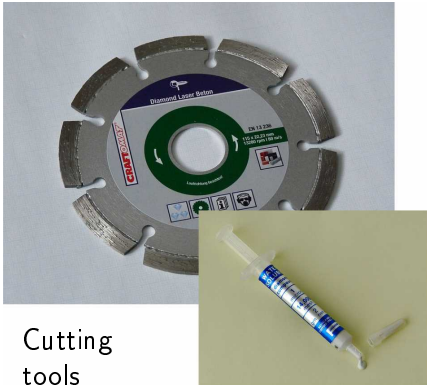
Big Hole (Kimberley mine), South Africa

**Natural**

about 30 000 ton per year

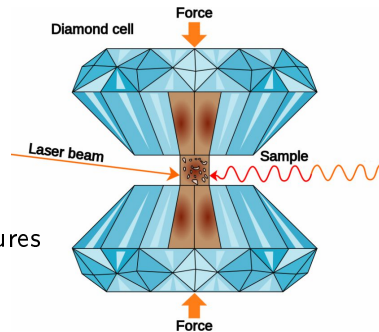
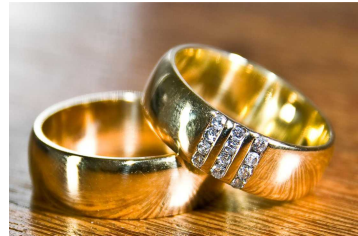
**Synthetic**  
about 1 200 ton per year



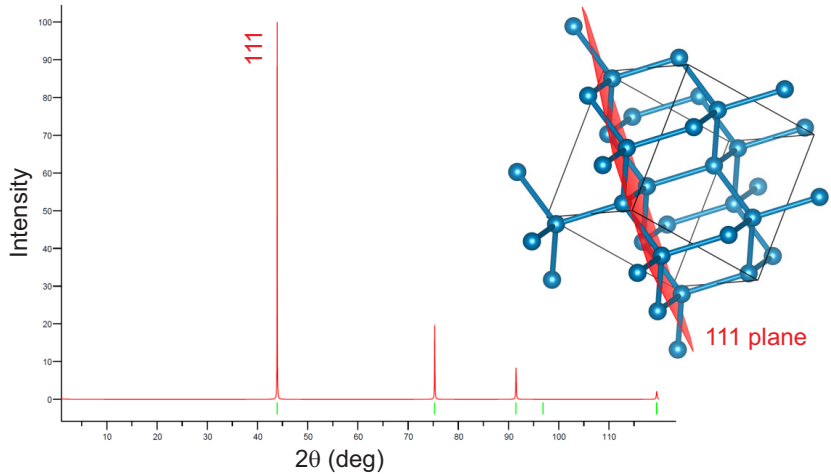


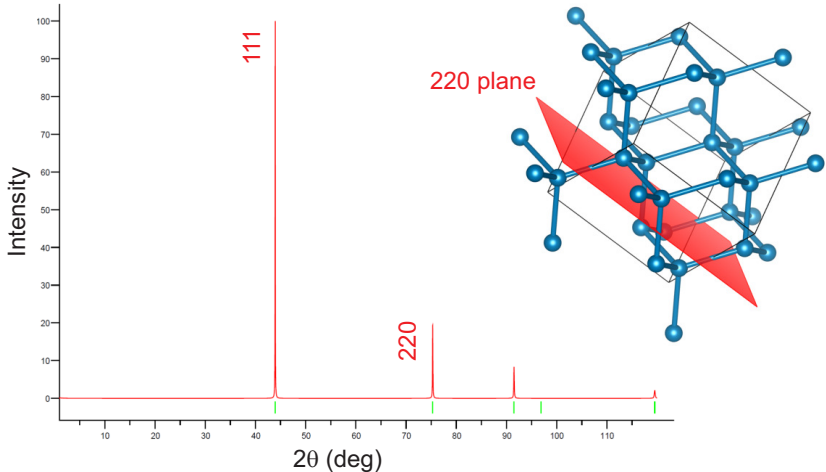
Cutting tools

Diamond is the **hardest** material known



# Problem of lattice planes





Lattice planes may not contain any atoms, yet they scatter x-rays