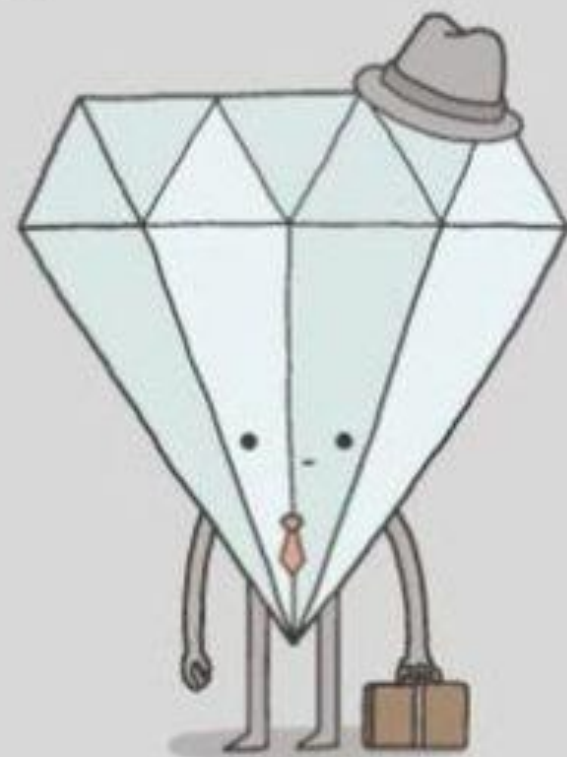
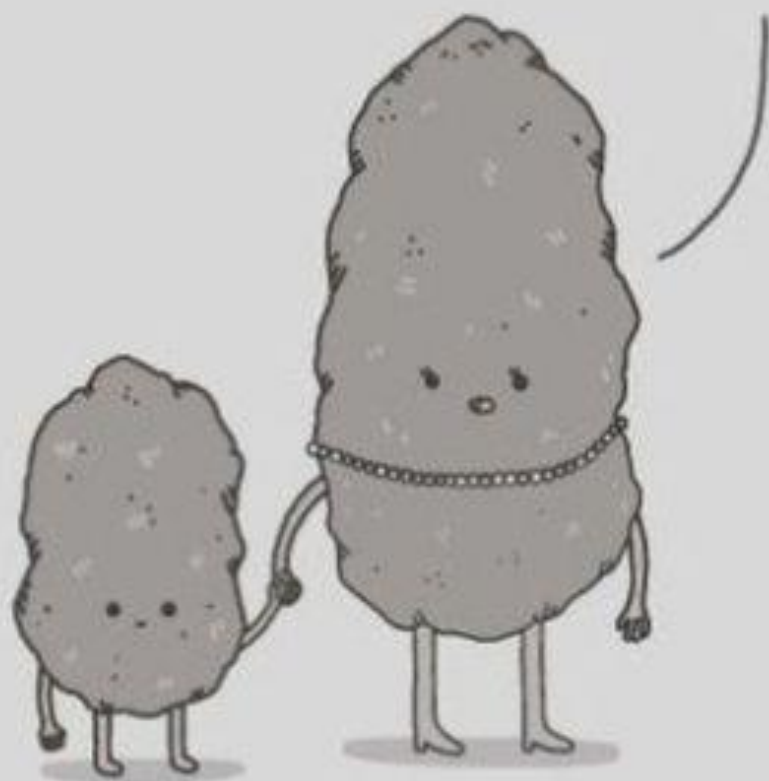


I can tell.

YOUR DAD'S BEEN
UNDER A LOT OF
PRESSURE LATELY.



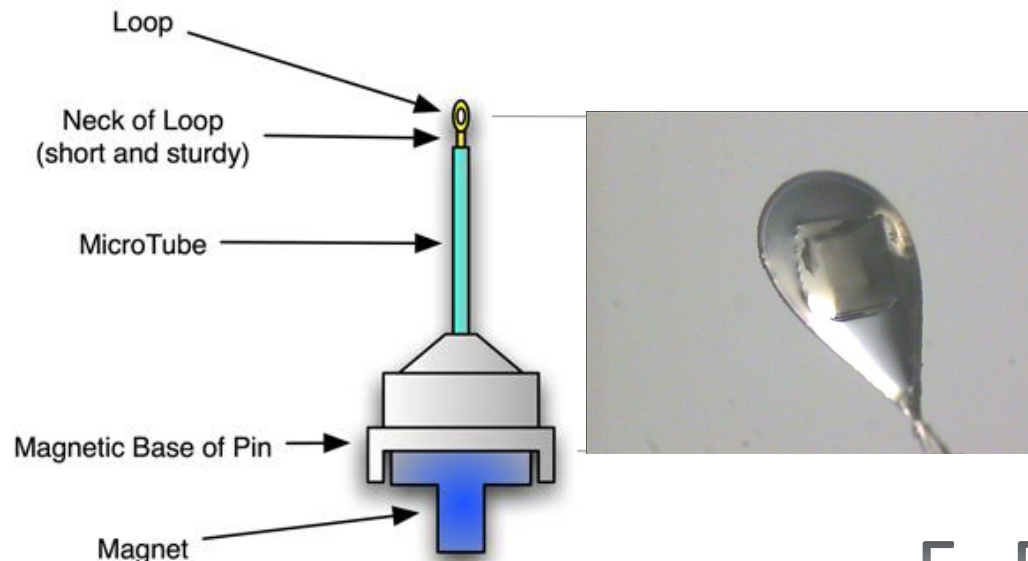


1. Make Crystal

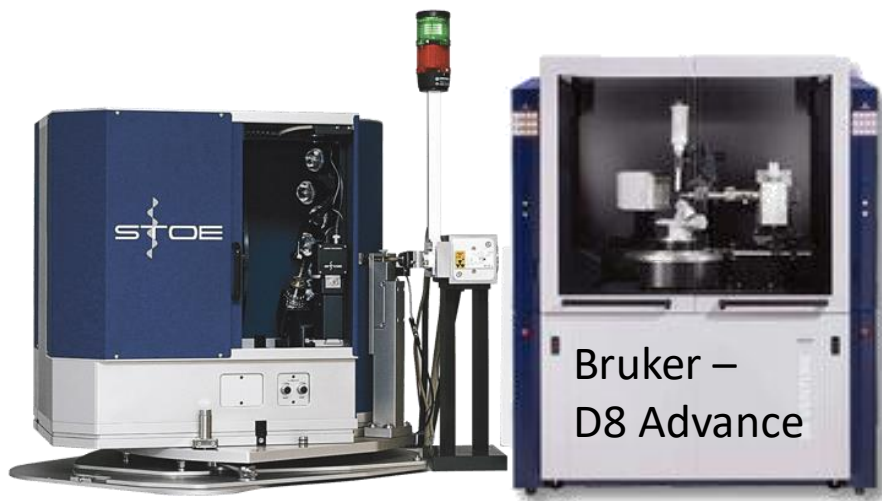


2. Choose Crystal

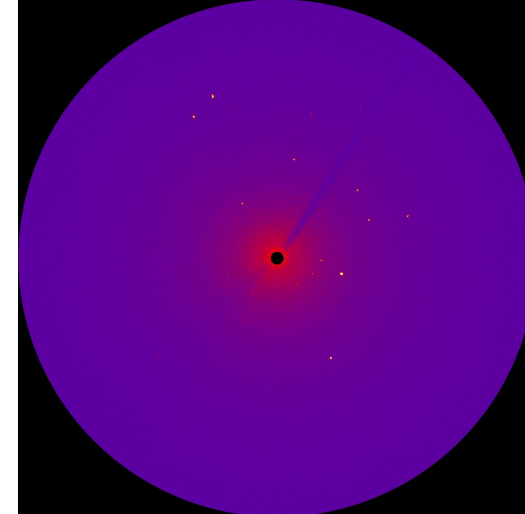
STOE – IPDS
(Image Plate Detector System)



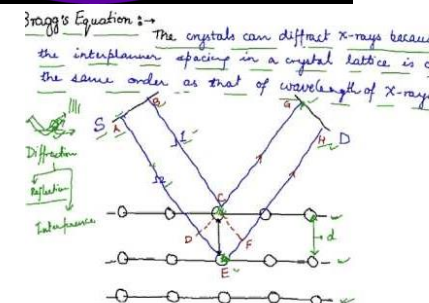
3. Mount Crystal



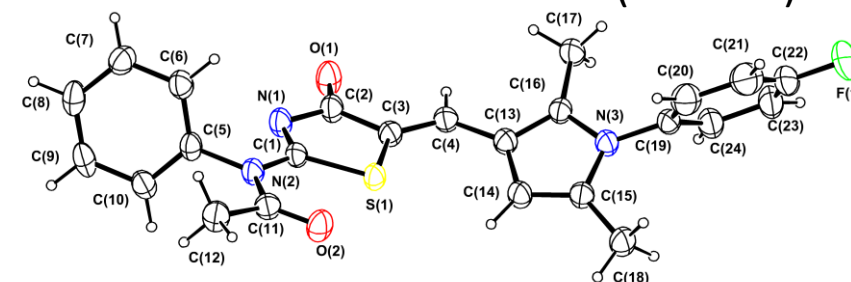
4. Measure crystal

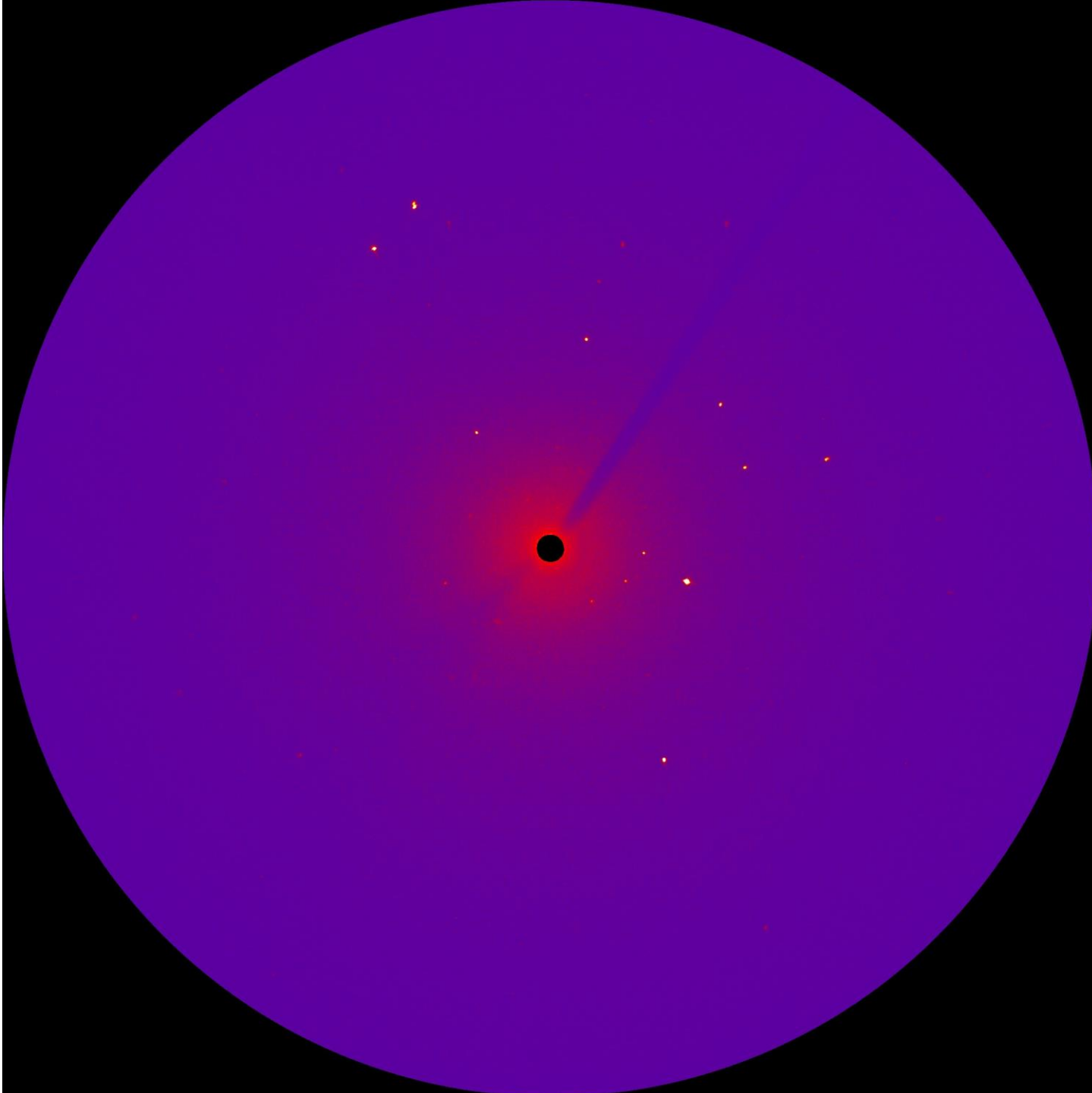


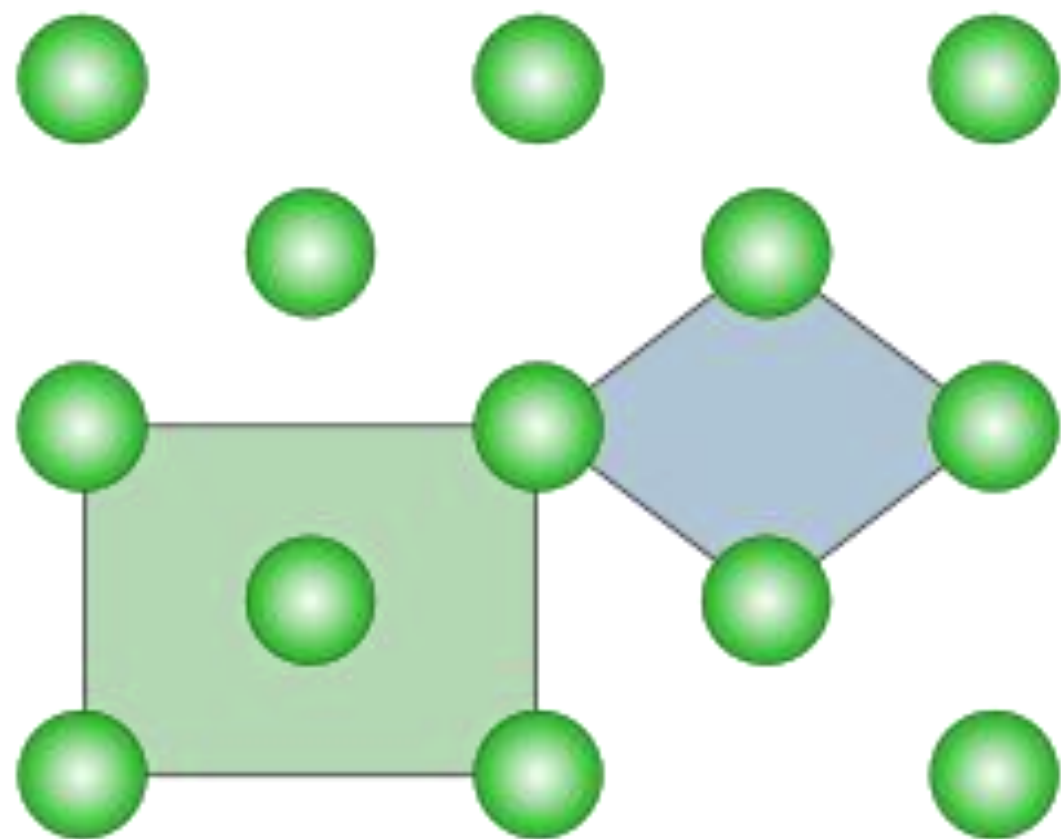
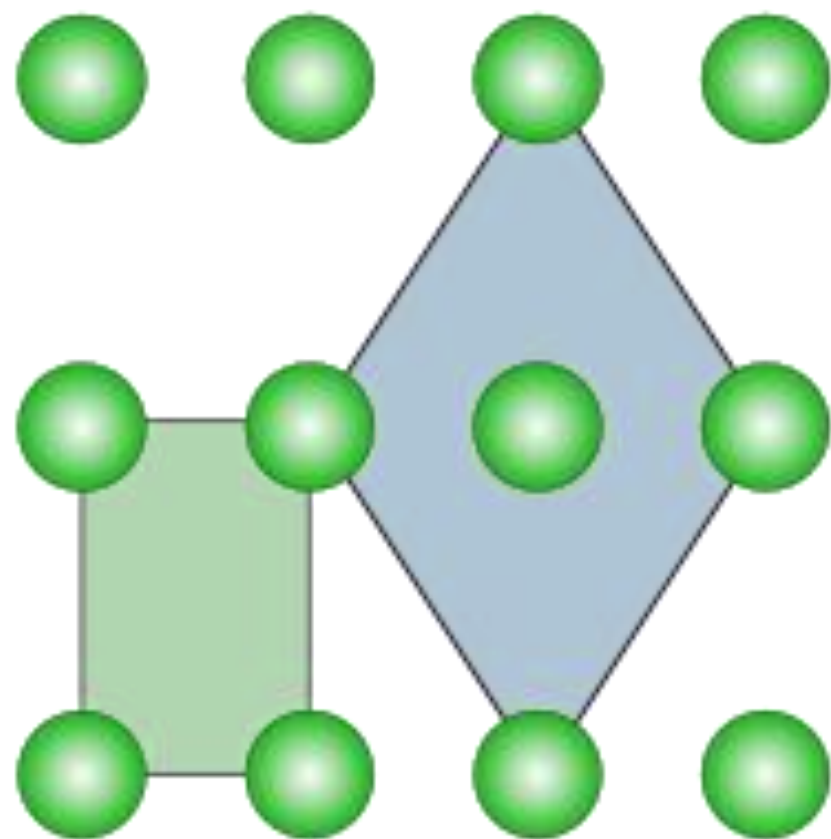
5. Data Reduction And Refinement



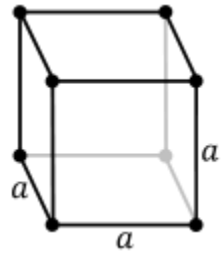
Math
Intuition
Experience
(Voodoo)



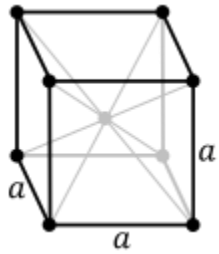




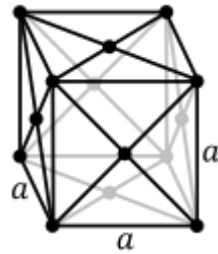
14 Bravais Lattices



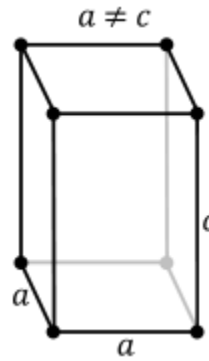
cP



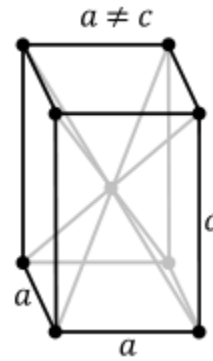
cI



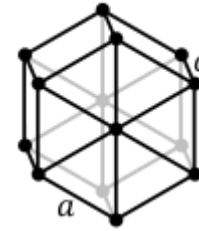
cF



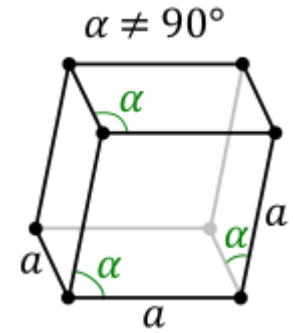
tP



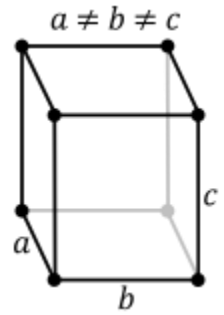
tI



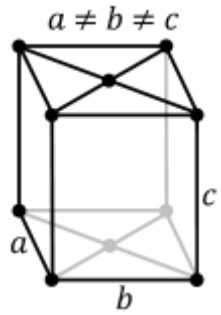
hP



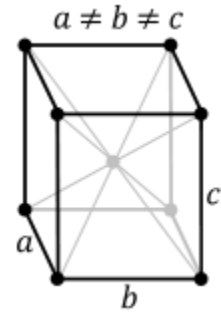
hR



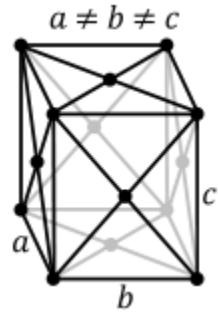
oP



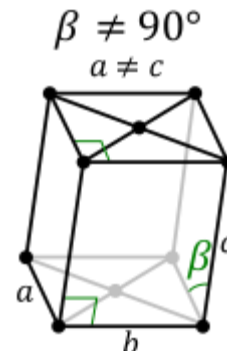
oC



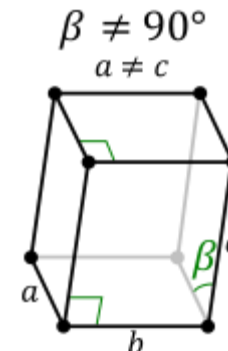
oI



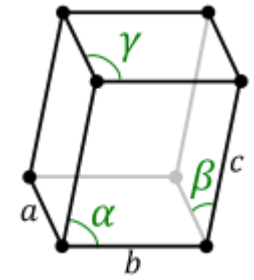
oF



mC

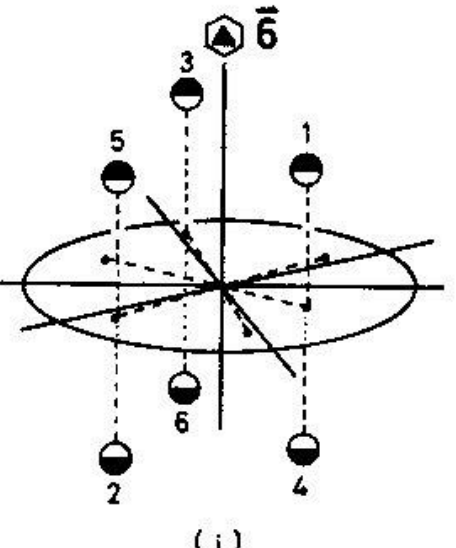
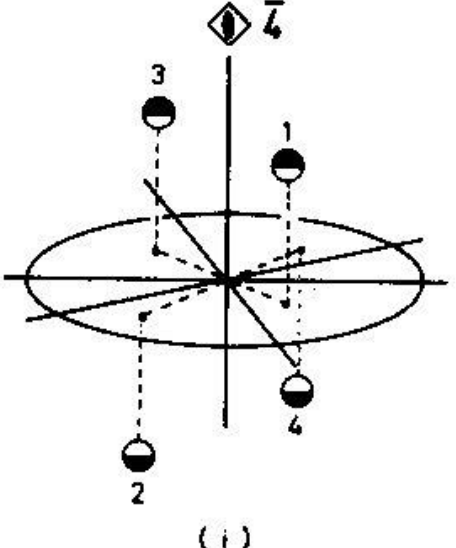
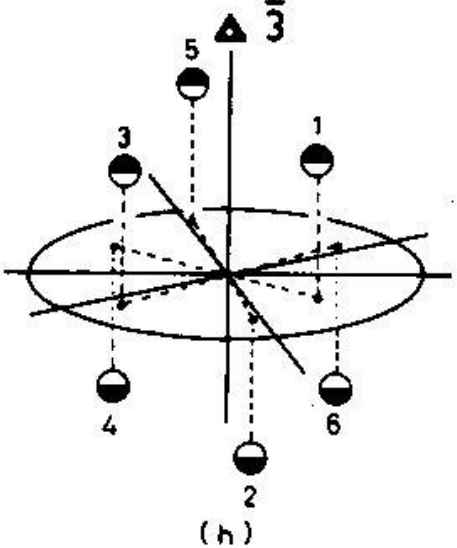
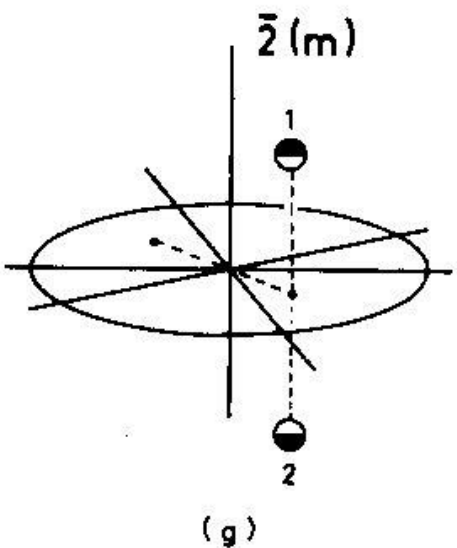
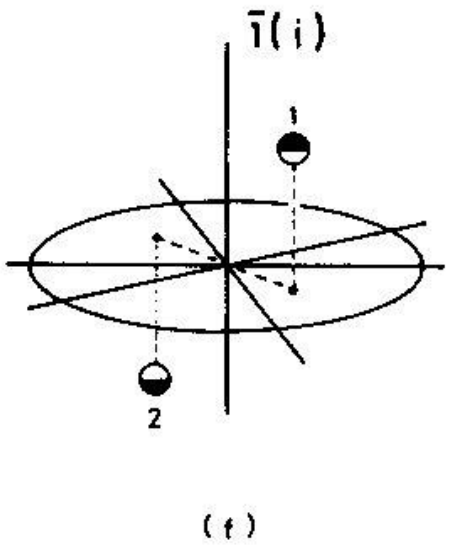
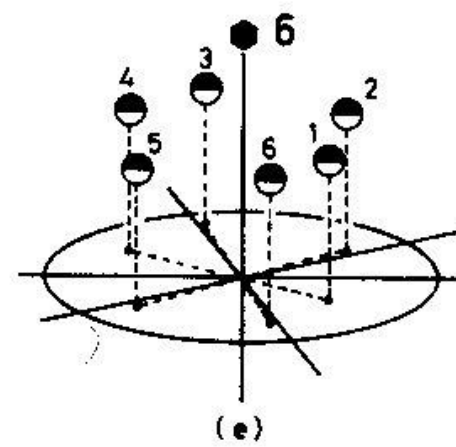
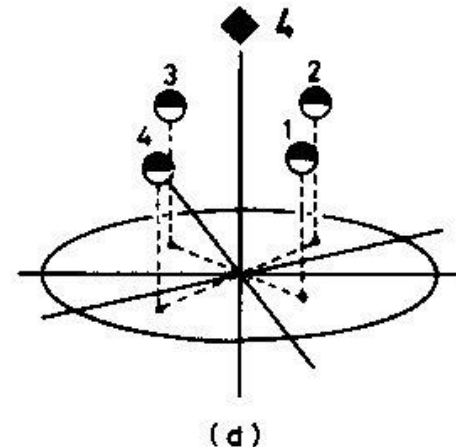
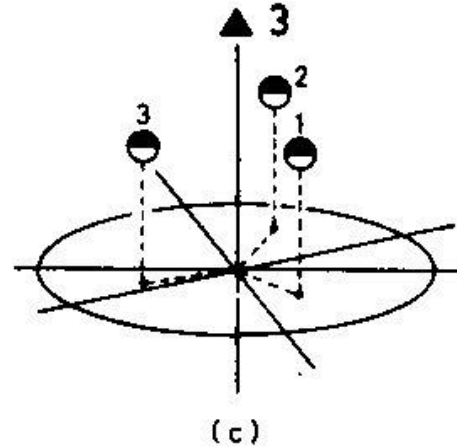
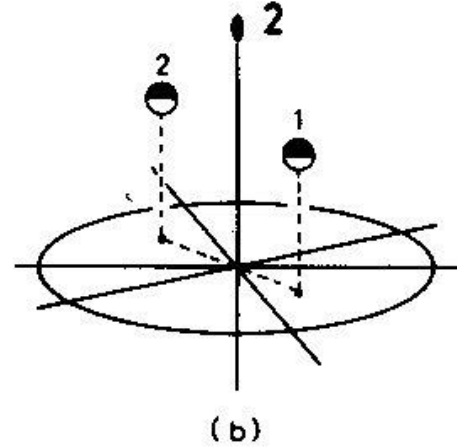
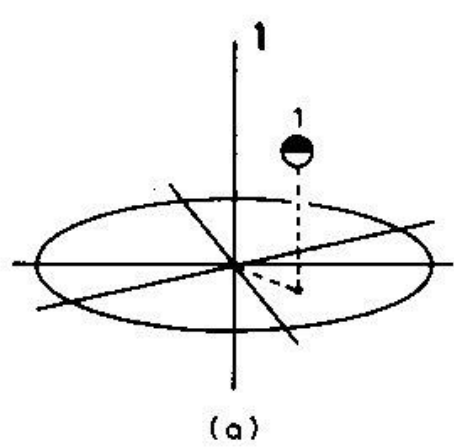


mP

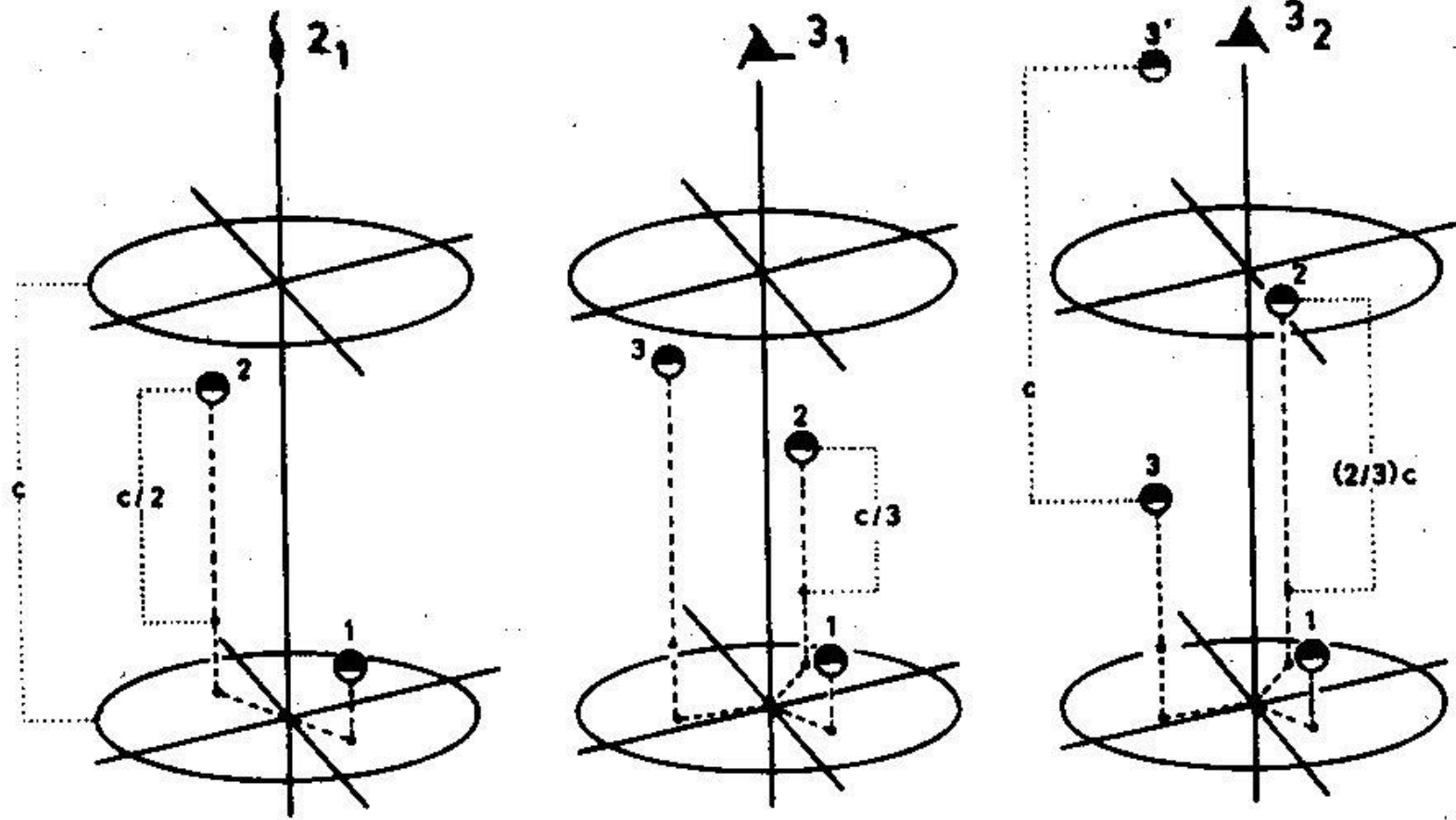


aP

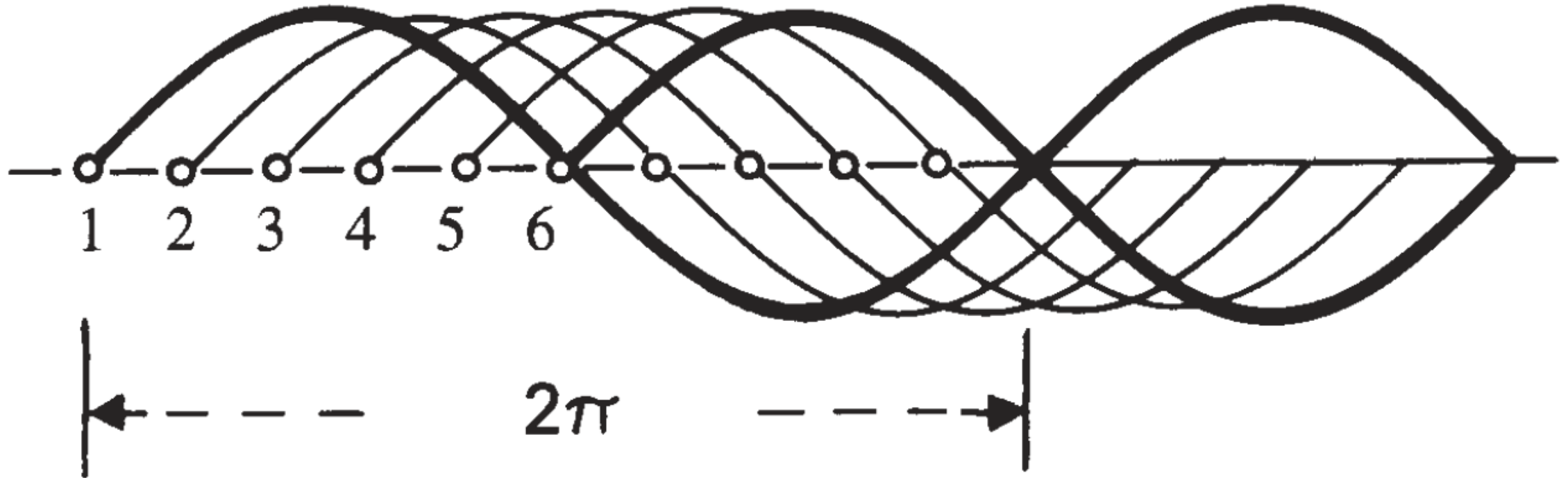
Hermann-Mauguin



Screw axis



$$\Delta = \lambda/10$$



P n m a

D_{2h}^{16}

m m m

Orthorhombic

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

No. 62

$P 2_1/n 2_1/m 2_1/a$

Patterson symmetry *P m m m*

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

General:

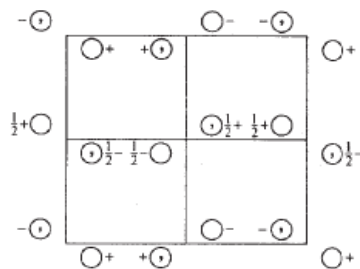
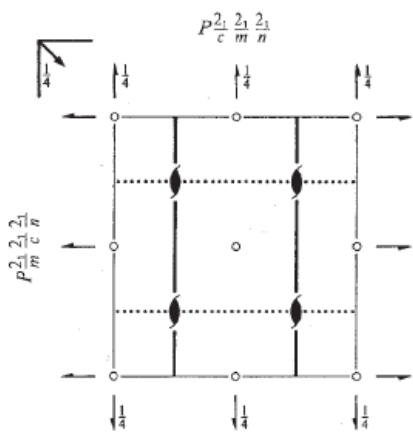
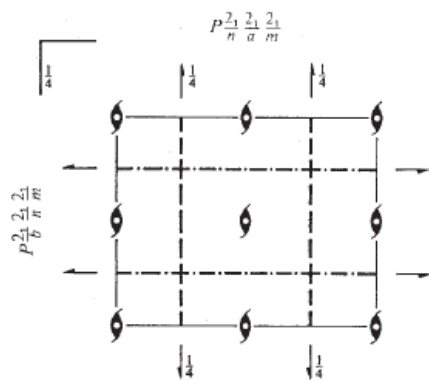
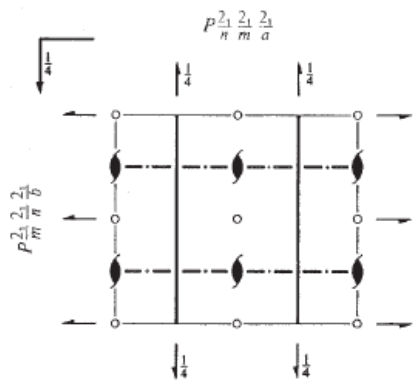
$Ok\bar{l} : k+l=2n$
 $hk0 : h=2n$
 $h00 : h=2n$
 $0k0 : k=2n$
 $00l : l=2n$

Special: as above, plus

no extra conditions

$hkl : h+l, k=2n$

$hkl : h+l, k=2n$



8	<i>d</i>	1	(1) x, y, z	(2) $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$	(3) $\bar{x}, y+\frac{1}{2}, \bar{z}$	(4) $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}+\frac{1}{2}$
			(5) $\bar{x}, \bar{y}, \bar{z}$	(6) $x+\frac{1}{2}, y, \bar{z}+\frac{1}{2}$	(7) $x, \bar{y}+\frac{1}{2}, z$	(8) $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$

4	<i>c</i>	\bar{m}	$x, \frac{1}{2}, z$	$\bar{x}+\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}$	$\bar{x}, \frac{1}{2}, \bar{z}$	$x+\frac{1}{2}, \frac{1}{2}, \bar{z}+\frac{1}{2}$
4	<i>b</i>	$\bar{1}$	$0, 0, \frac{1}{2}$	$\frac{1}{2}, 0, 0$	$0, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}, 0$
4	<i>a</i>	$\bar{1}$	$0, 0, 0$	$\frac{1}{2}, 0, \frac{1}{2}$	$0, \frac{1}{2}, 0$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Symmetry of special projections

Along [001] $p 2gm$
 $a'=\frac{1}{2}a$ $b'=b$
Origin at $0, 0, z$

Along [100] $c 2mm$
 $a'=b$ $b'=c$
Origin at $x, \frac{1}{2}, \frac{1}{2}$

Along [010] $p 2gg$
 $a'=c$ $b'=a$
Origin at $0, y, 0$

Maximal non-isomorphic subgroups

I	$[2]P 2_1 2_1 2_1$	1; 2; 3; 4
	$[2]P 1 1 2_1/a (P 2_1/c)$	1; 2; 5; 6
	$[2]P 1 2_1/m 1 (P 2_1/m)$	1; 3; 5; 7
	$[2]P 2_1/n 1 1 (P 2_1/c)$	1; 4; 5; 8
	$[2]P n m 2_1 (P m n 2_1)$	1; 2; 7; 8
	$[2]P n 2_1 a (P n a 2_1)$	1; 3; 6; 8
	$[2]P 2_1 m a (P m c 2_1)$	1; 4; 6; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc $[3]P n m a (a'=3a)$; $[3]P n m a (b'=3b)$; $[3]P n m a (c'=3c)$

Minimal non-isomorphic supergroups

I none

II $[2]A m m a (C m c m)$; $[2]B b m m (C m c m)$; $[2]C c m b (C m c a)$; $[2]I m m a$; $[2]P n m m (2a'=a) (P m m n)$; $[2]P c m a (2b'=b) (P b a m)$; $[2]P b m a (2c'=c) (P b c m)$

Origin at $\bar{1}$ on $12_1 1$

Asymmetric unit $0 \leq x \leq \frac{1}{2}$; $0 \leq y \leq \frac{1}{2}$; $0 \leq z \leq 1$

Symmetry operations

- (1) $\bar{1}$
- (2) $2(0, 0, \frac{1}{2})$ $\frac{1}{2}, 0, z$
- (3) $2(0, \frac{1}{2}, 0)$ $0, y, 0$
- (4) $2(\frac{1}{2}, 0, 0)$ $x, \frac{1}{2}, \frac{1}{2}$
- (5) $\bar{1}$ $0, 0, 0$
- (6) a $x, y, \frac{1}{2}$
- (7) m $x, \frac{1}{2}, z$
- (8) $n(0, \frac{1}{2}, \frac{1}{2})$ $\frac{1}{2}, y, z$

Space group Symbolism according to Hermann-Mauguin

(Int.Tables for X-Ray Crystallography)

Kurzsymbol:

$I 4/m c m$

vollständiges Symbol:

$I \underbrace{4/m}_{\text{vierzählige Drehachse}} \underbrace{2/c}_{\text{Spiegelebene}} \underbrace{2/m}_{\text{Spiegelebene}}$

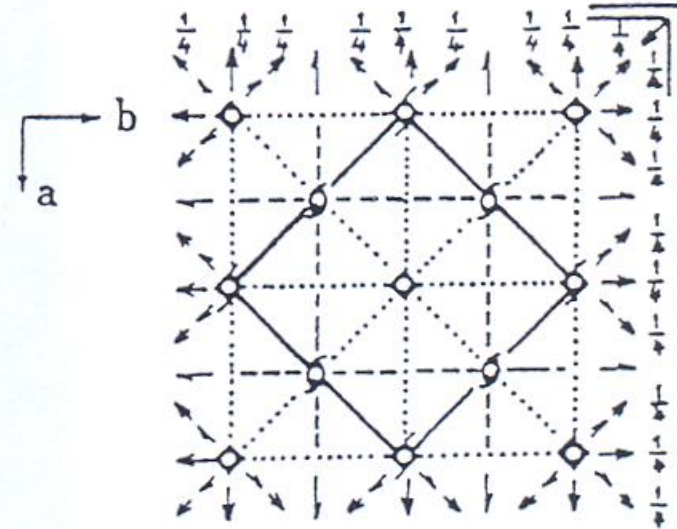
Bedeutung:

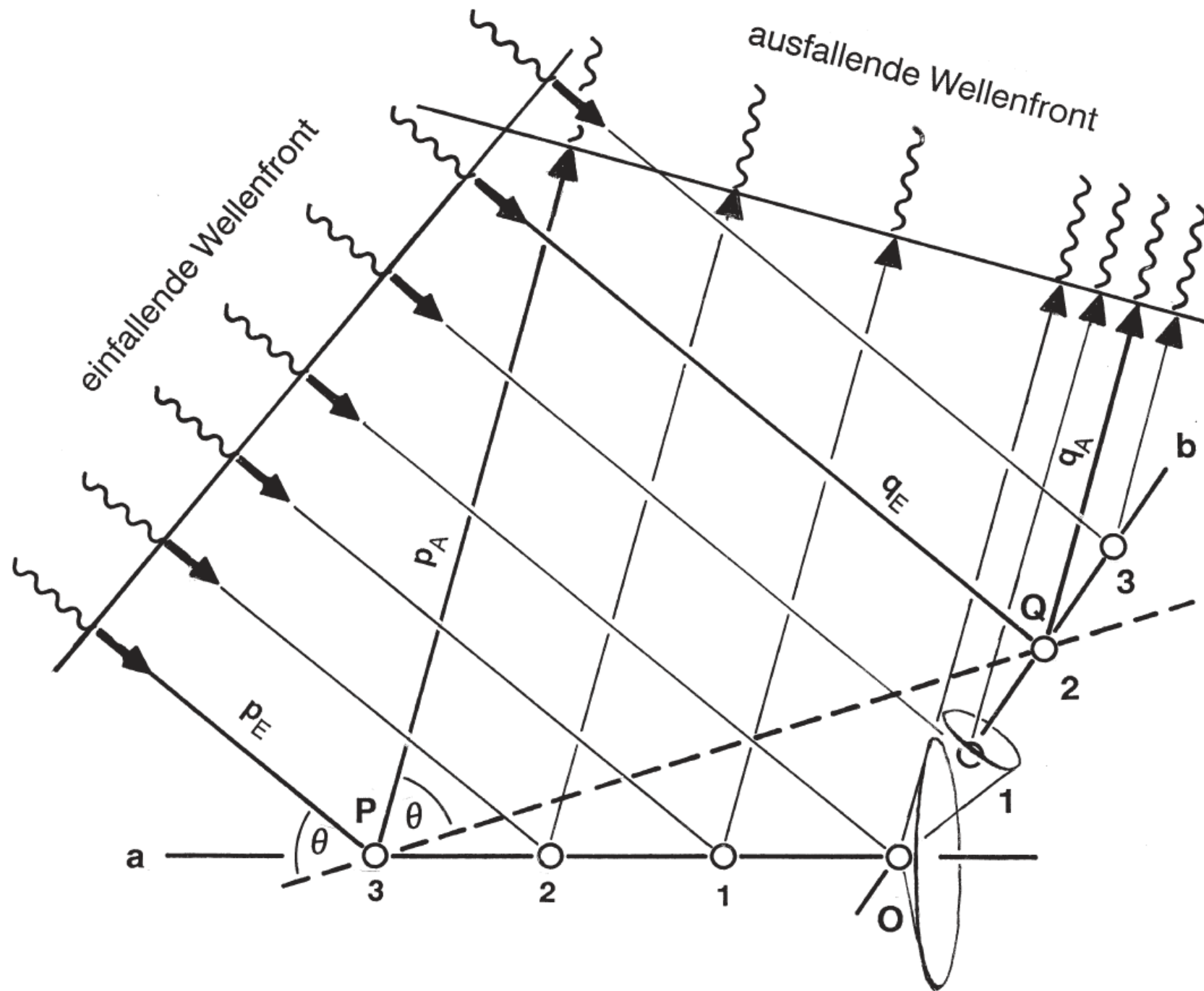
innen-
zentriertes
Gitter

vierzählige Drehachse in
Richtung c, Spiegelebene
senkrecht dazu

zweizählige Drehachse in Richtung
 $d = a+b$, Spiegelebene senkrecht dazu

zweizählige Drehachse in Richtung a, Gleitspiegel-
ebene mit Gleitrichtung c senkrecht zu a





Monoklin

$$\sin^2 \theta = \frac{\lambda^2}{4} \left[\frac{h^2}{a^2 \sin^2 \beta} + \frac{k^2}{b^2} + \frac{l^2}{c^2 \sin^2 \beta} - \frac{2hl \cos \beta}{ac \sin^2 \beta} \right]$$

Orthorhombisch

$$\sin^2 \theta = \frac{\lambda^2}{4} \left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]$$

Tetragonal

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} \left[h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2 \right]$$

Hexagonal und trigonal

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} \left[\frac{4}{3} (h^2 + k^2 + hk) + \left(\frac{a}{c}\right)^2 l^2 \right]$$

Kubisch

$$\sin^2 \theta = \frac{\lambda^2}{4a^2} \left[h^2 + k^2 + l^2 \right]$$

Triklin

$$\sin^2 \theta = \frac{\lambda^2}{4} [h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2klb^*c^* \cos \alpha^* + 2lhc^*a^* \cos \beta^* + 2hka^*b^* \cos \gamma^*]$$

$$a^* = \frac{1}{V} bc \sin \alpha, \quad \cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}$$

$$b^* = \frac{1}{V} ca \sin \beta, \quad \cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}$$

$$c^* = \frac{1}{V} ab \sin \gamma, \quad \cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$$

$$V = abc \sqrt{1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma}$$



Schrödinger's Lunchbox.