# Basics of Macromolecular Crystallography

## 06 Symmetry and Space Groups

Andrea Thorn

**Zoom** Mondays 16:00 Berlin time

Register at lecture@thorn-lab.de

macromolecular_crystallography

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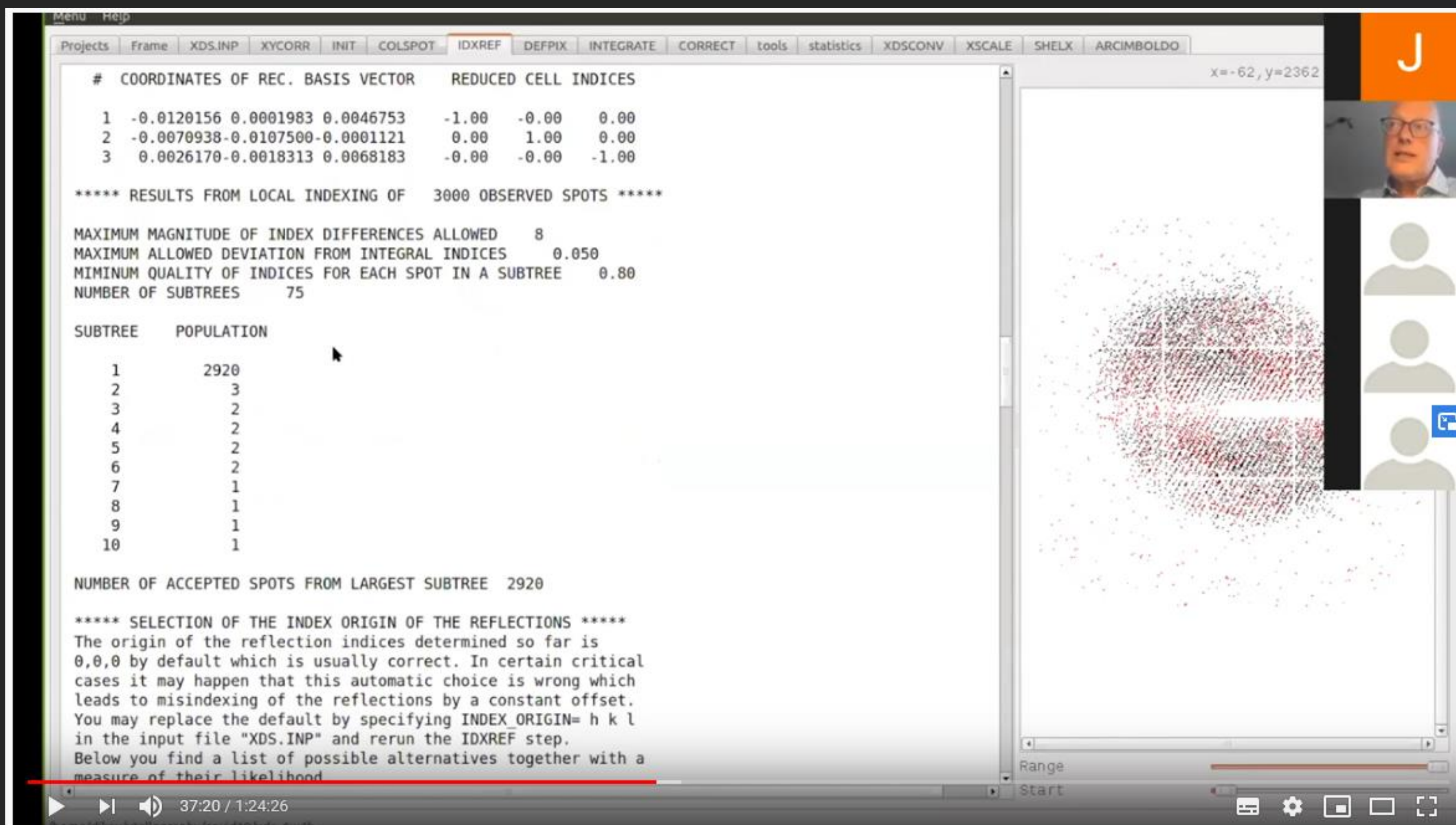
# You would like to know more about practical data processing?

Watch: **Kay Diederichs - XDS and XDSGUI** (SBGRID)
https://www.youtube.com/watch?v=3WU9NrILECo



# Symmetry

Andrea Thorn

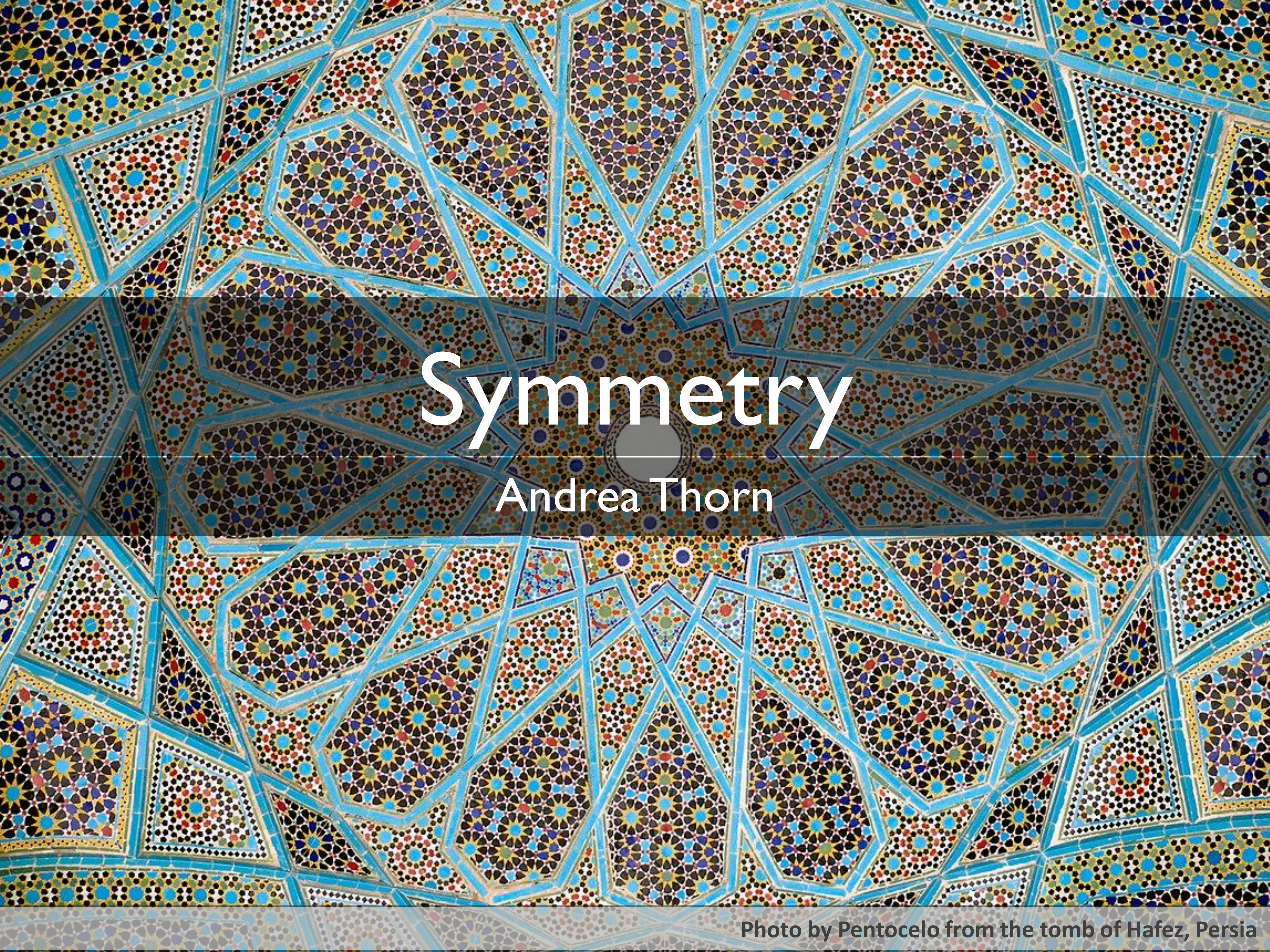
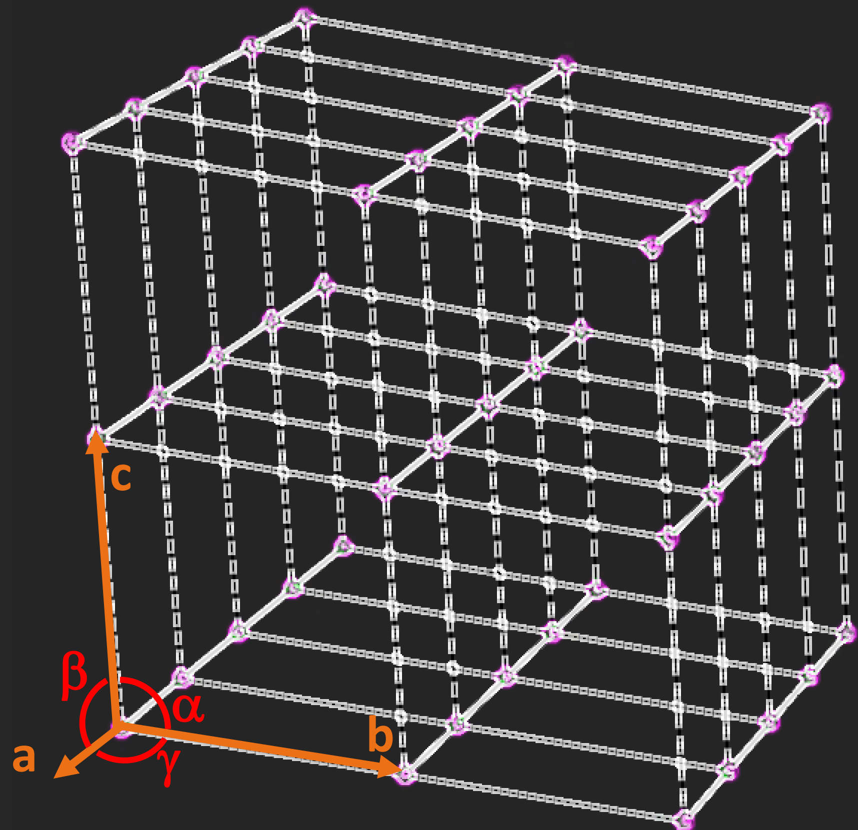


Photo by Pentocelo from the tomb of Hafez, Persia

# Definition: Crystal

A **crystal** is a solid material whose constituents, such as atoms, molecules or ions, are arranged in a highly ordered microscopic structure, forming a **crystal lattice** that extends in all directions.

Crystals are made up of identical 'bricks' (unit-cells) that constitute a three-dimensional translation lattice. The cell is defined by the 3 vectors a, b and c; the 3 angles between them are $\alpha$, $\beta$ and $\gamma$ as shown in the diagram.

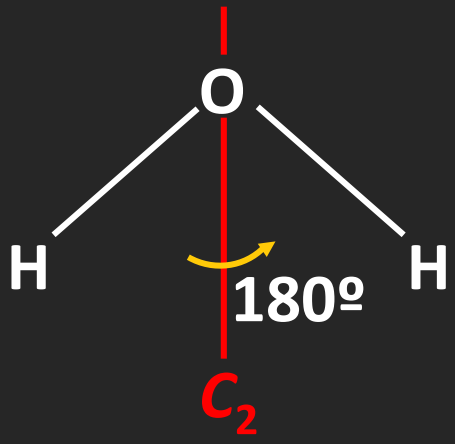



Pictures courtesy of George Sheldrick

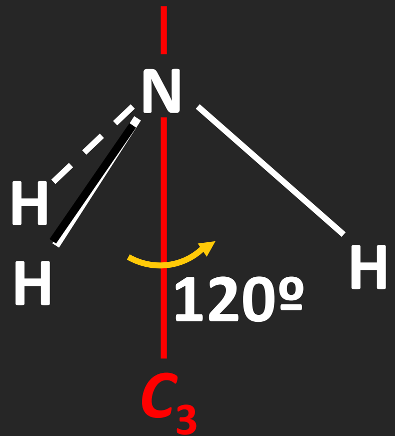
Point groups, plane groups

# SYMMETRY OPERATIONS & UNIT CELL

# Point groups:




- C2 rotation axis along the angle bisector
- two mirror planes that intersect each other along the rotation axis
- each combination of two of these elements would generate the third.
- point group: **C2v** or **2mm**

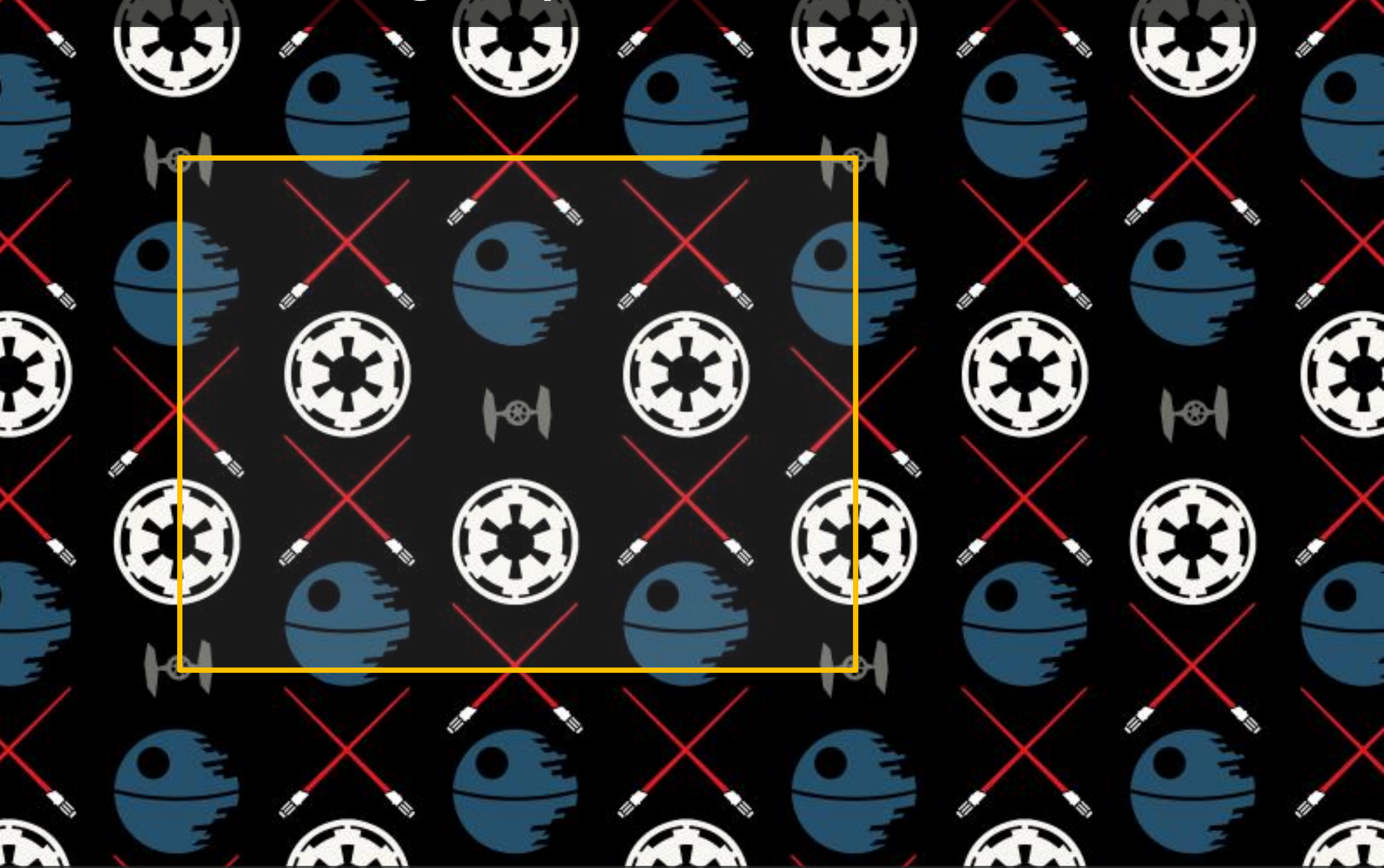



- C3 rotation axis
- three mirror planes that intersect one another along the rotation axis.
- point group: **C3v** or **3m**

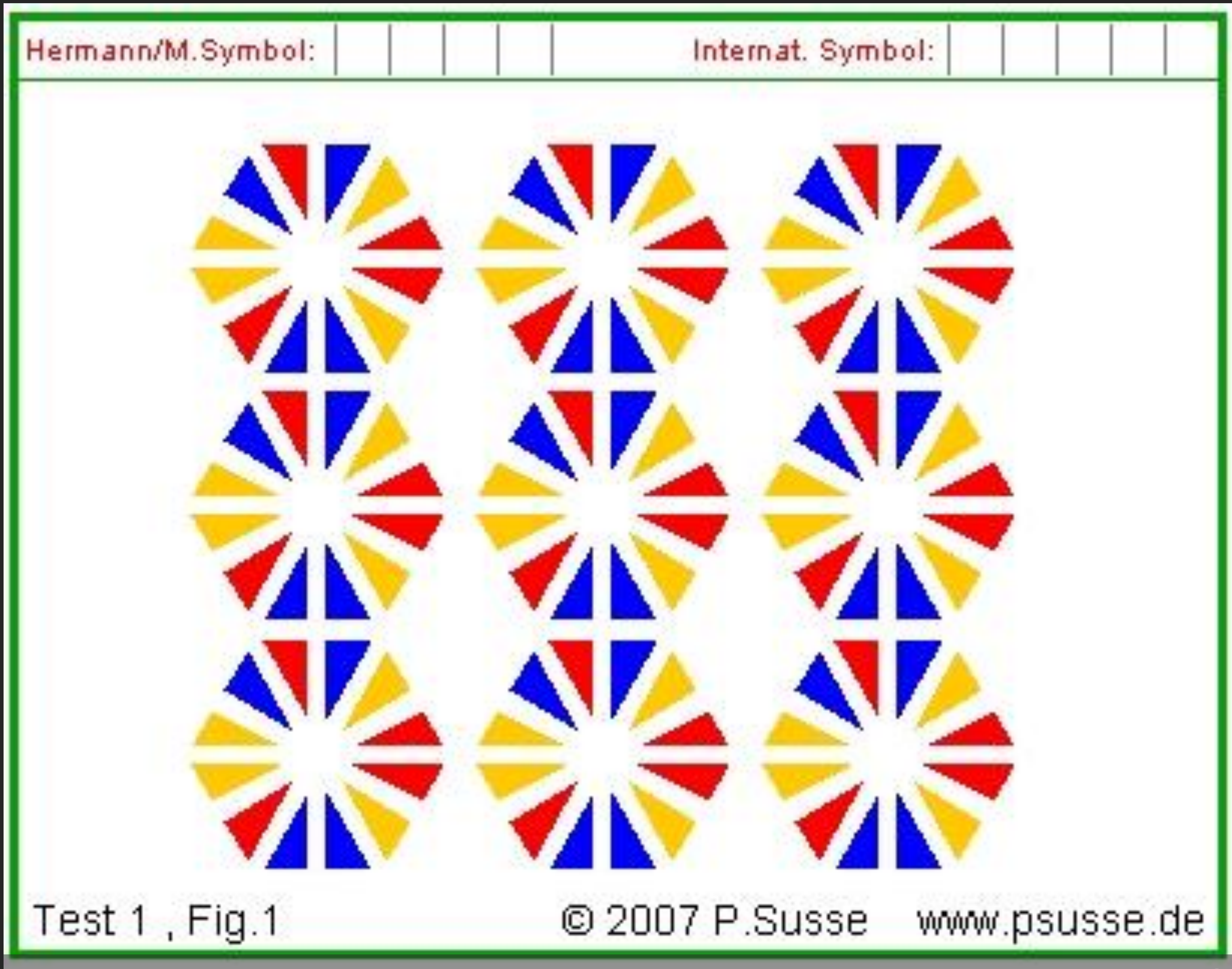
http://symmetry.otterbein.edu/

Have a look at: http://symmetry.otterbein.edu/! Pictures courtesy of George Sheldrick

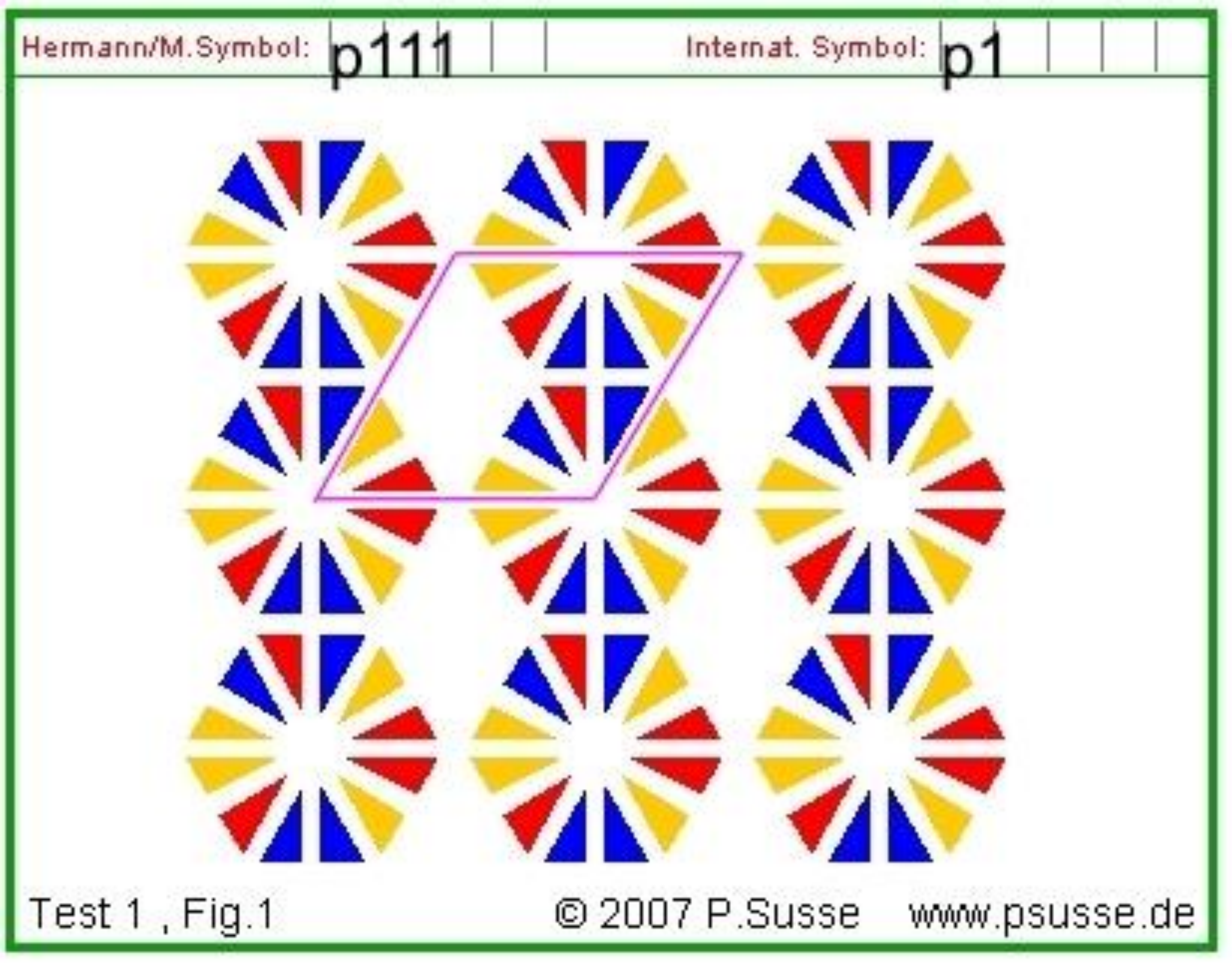
# Plane groups - The easiest case:



Design by Keith Greenstein

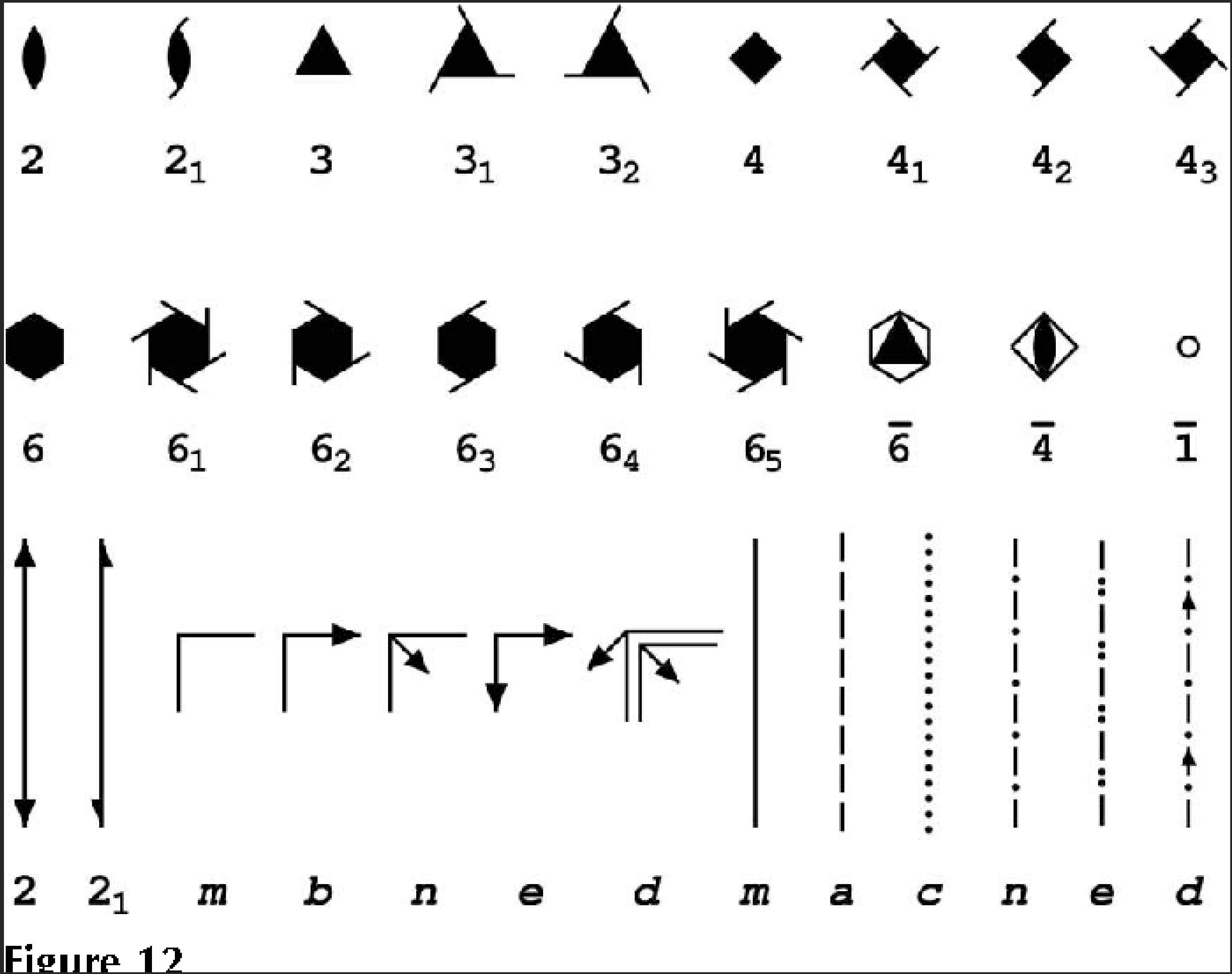



Courtesy of P. Susse



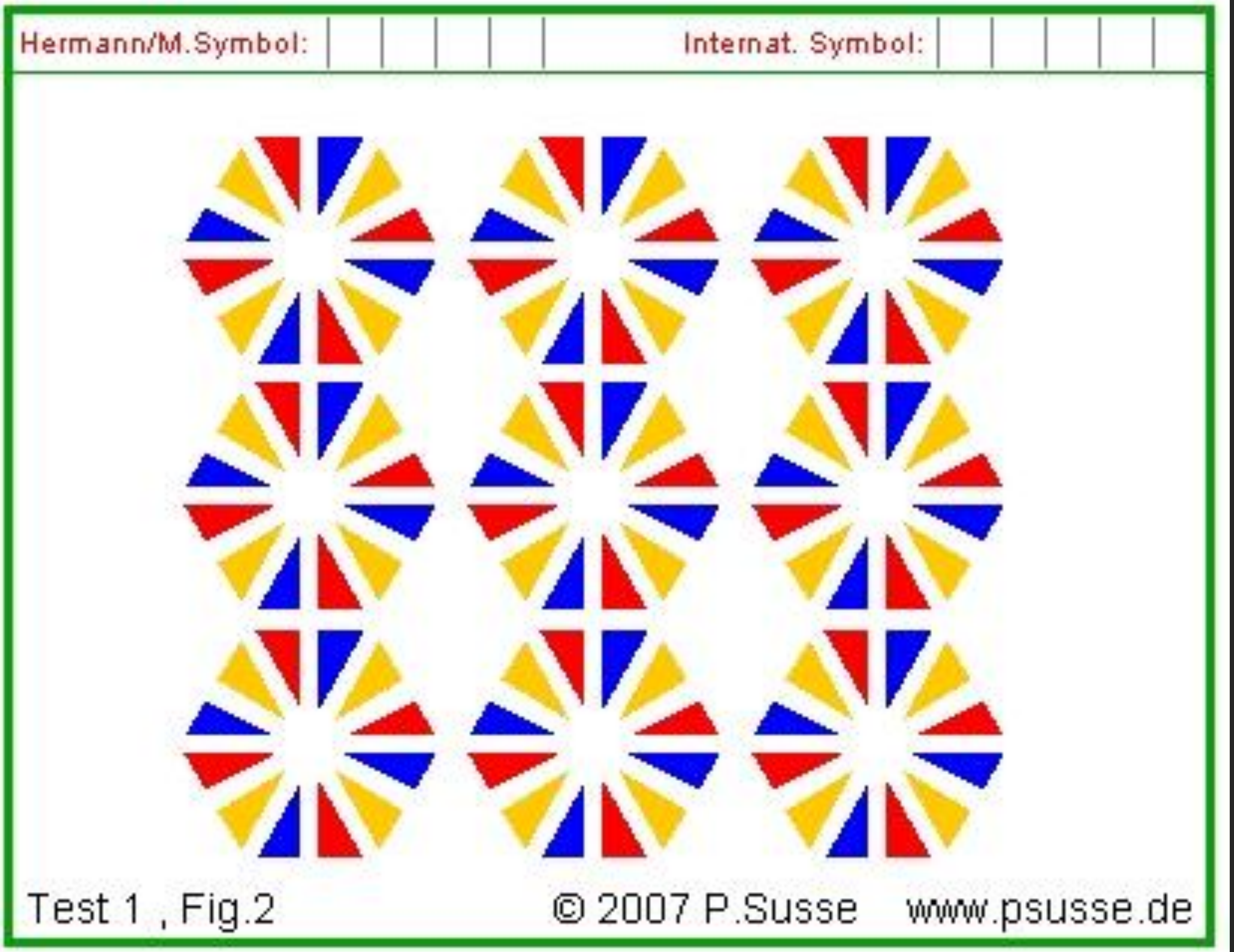

Courtesy of P. Susse

# Symmetry operations

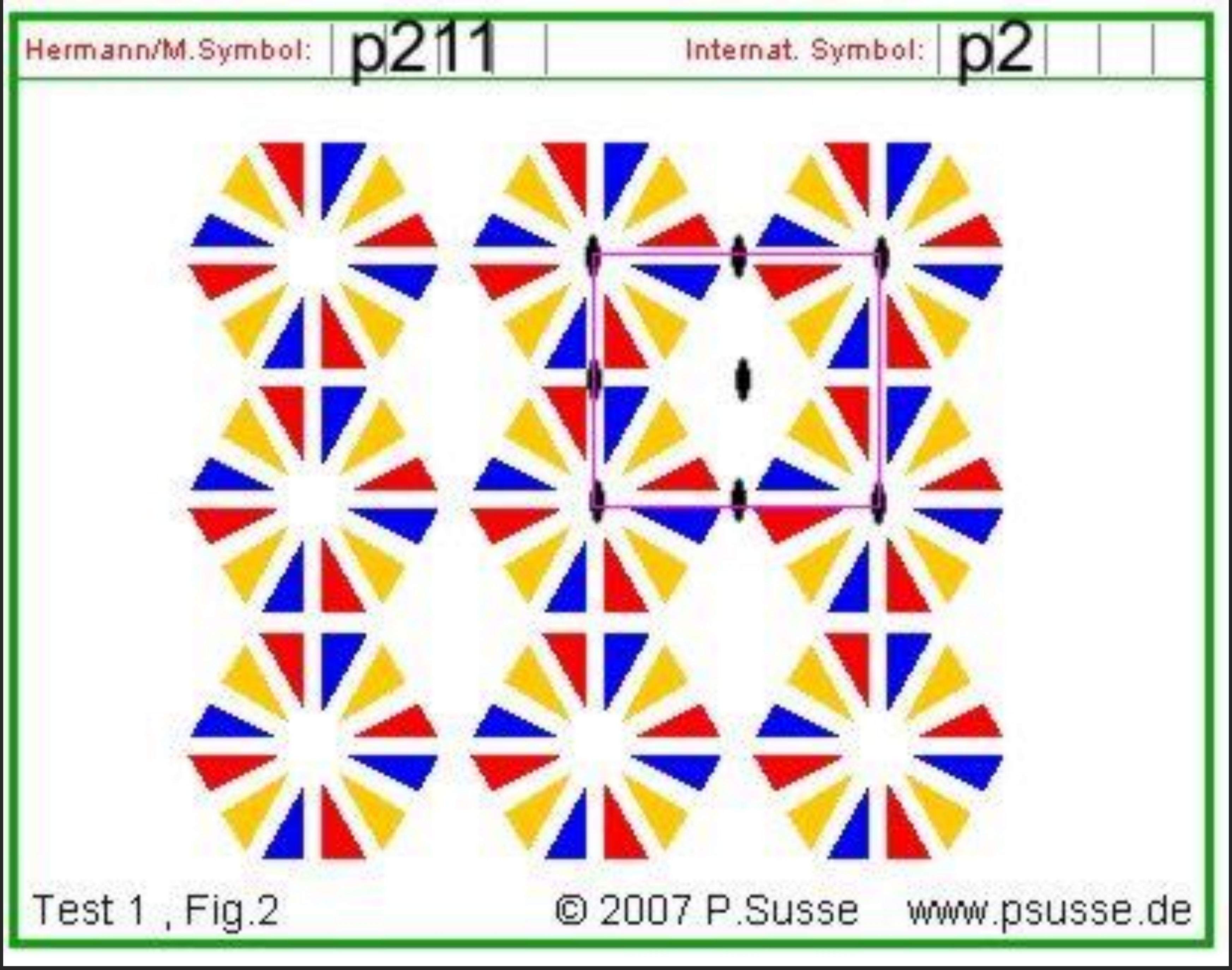



Dauter, Z. & Jaskolski M. (2010) J. Appl. Cryst. 43, 1150–1171

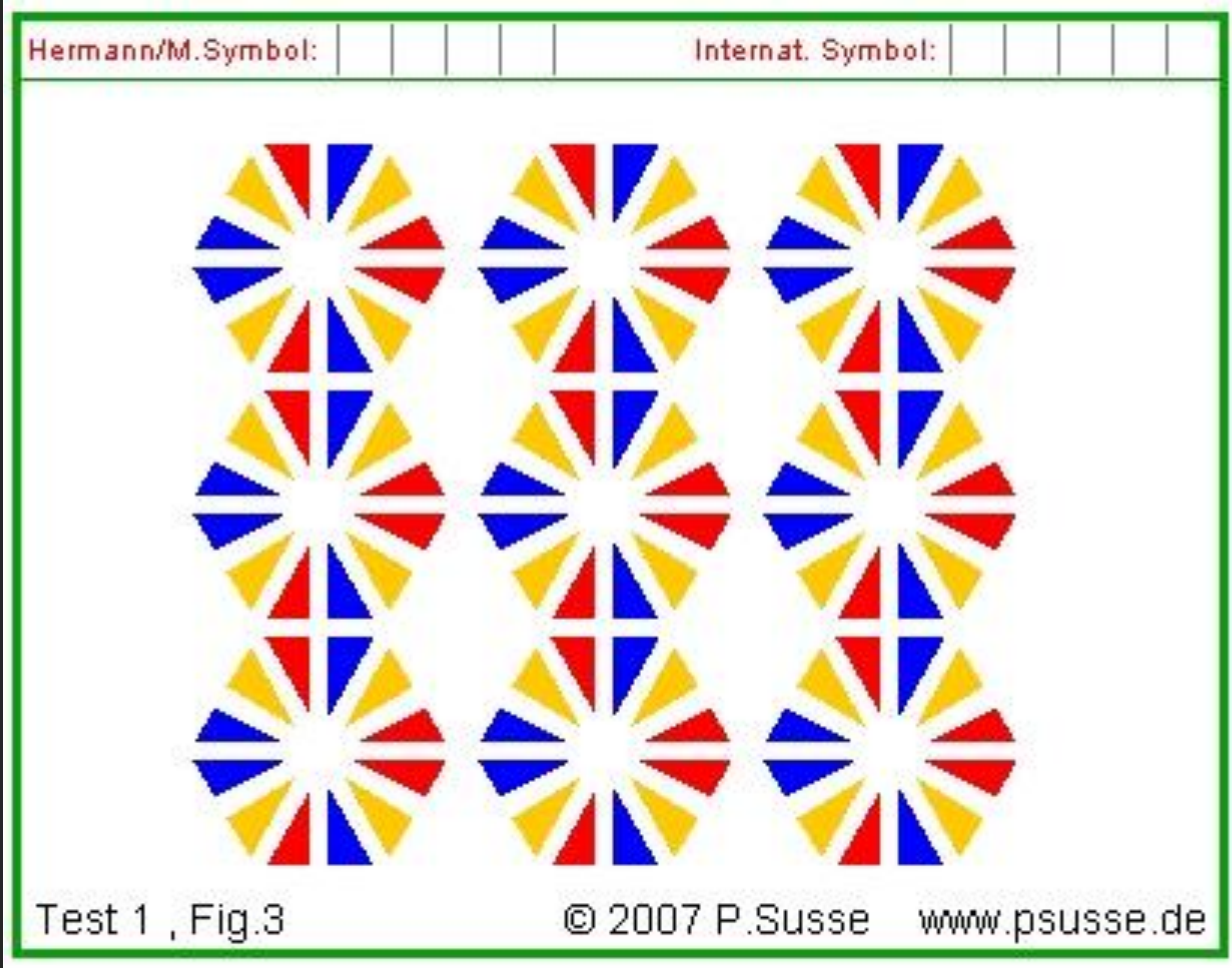
"How to read (and understand) Volume A of International Tables for Crystallography: an introduction for nonspecialists"



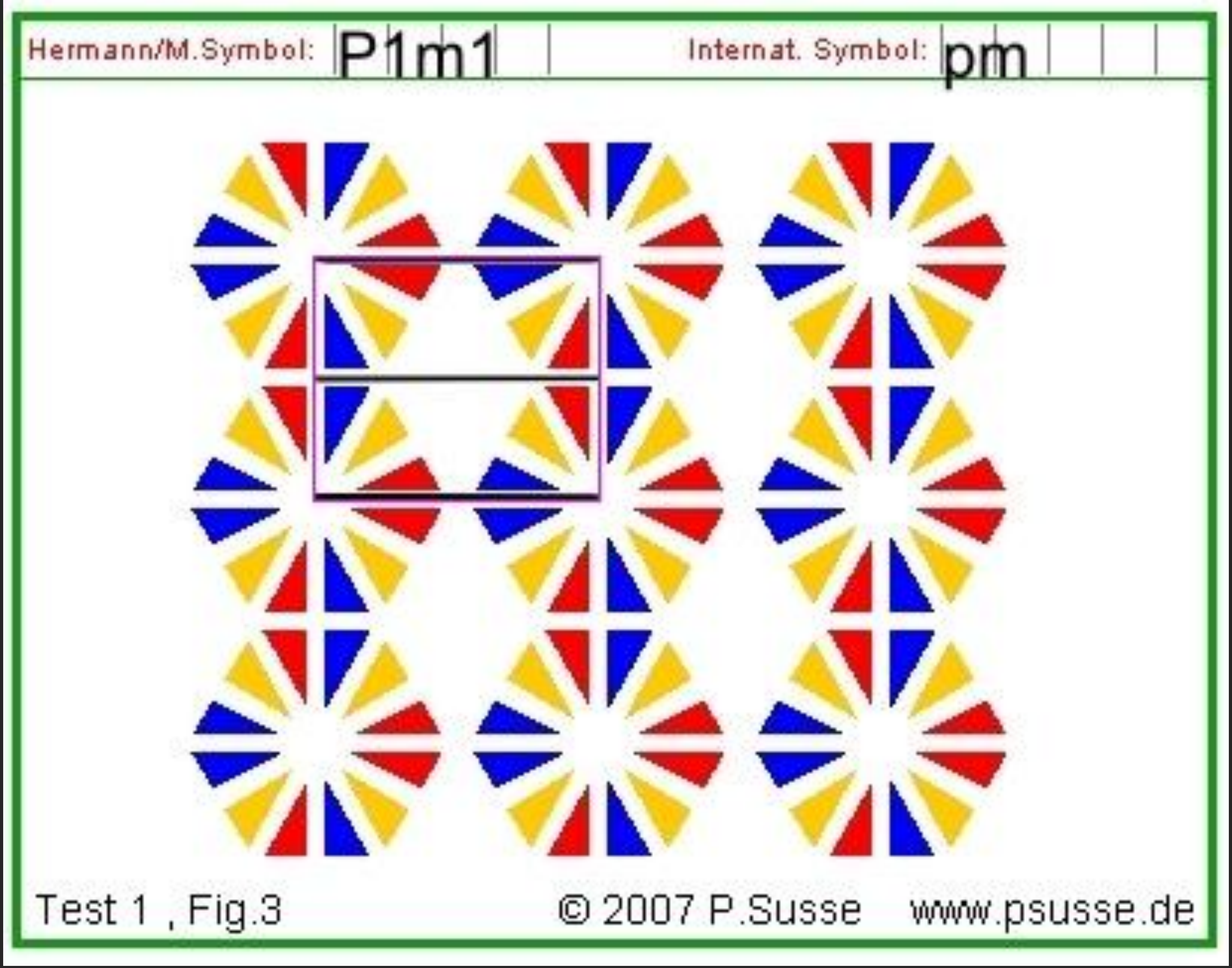

Courtesy of P. Susse



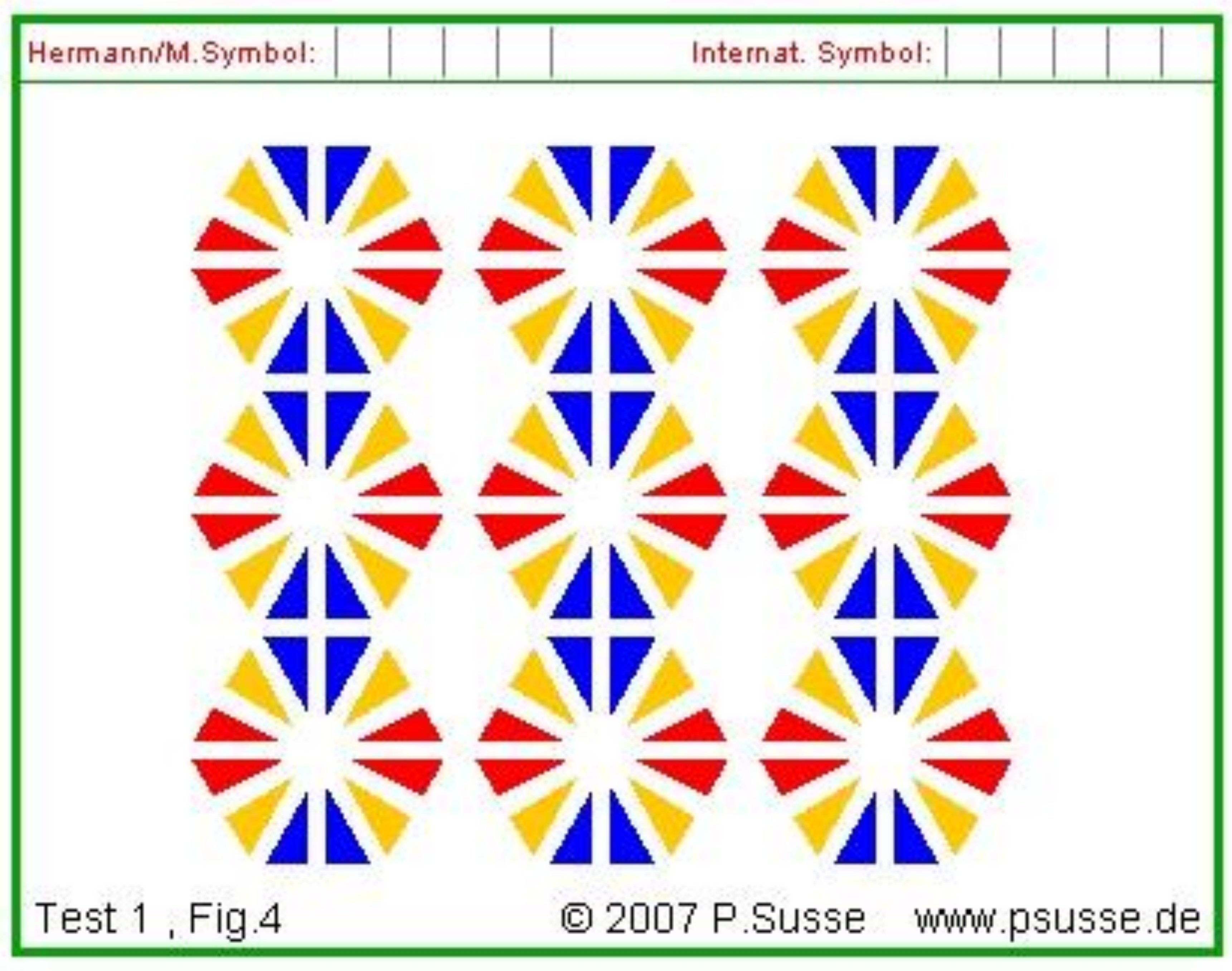

Courtesy of P. Susse



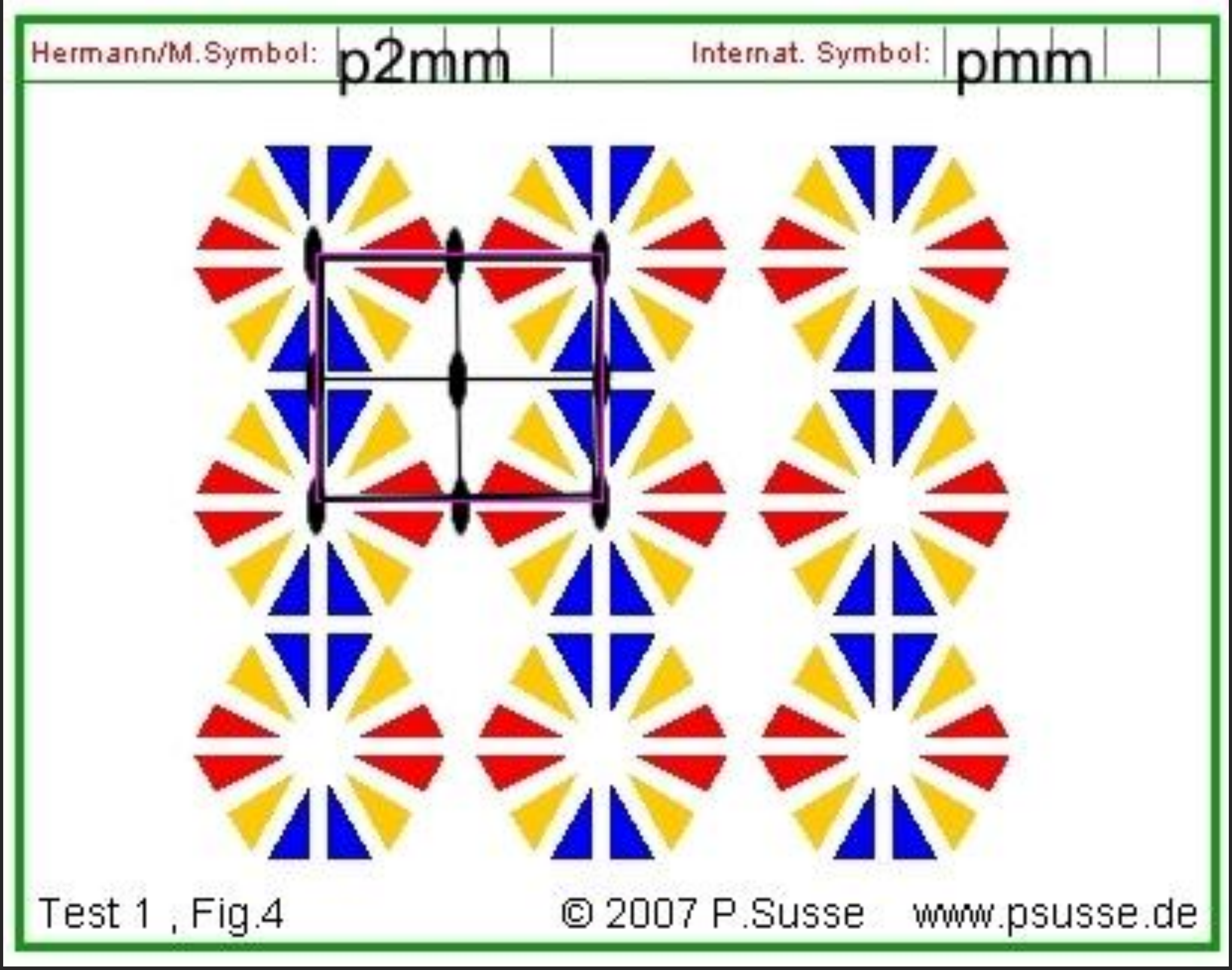

Courtesy of P. Susse




Courtesy of P. Susse




Courtesy of P. Susse




Courtesy of P. Susse

This is not nearly complicated enough

# BRAVAIS LATTICES

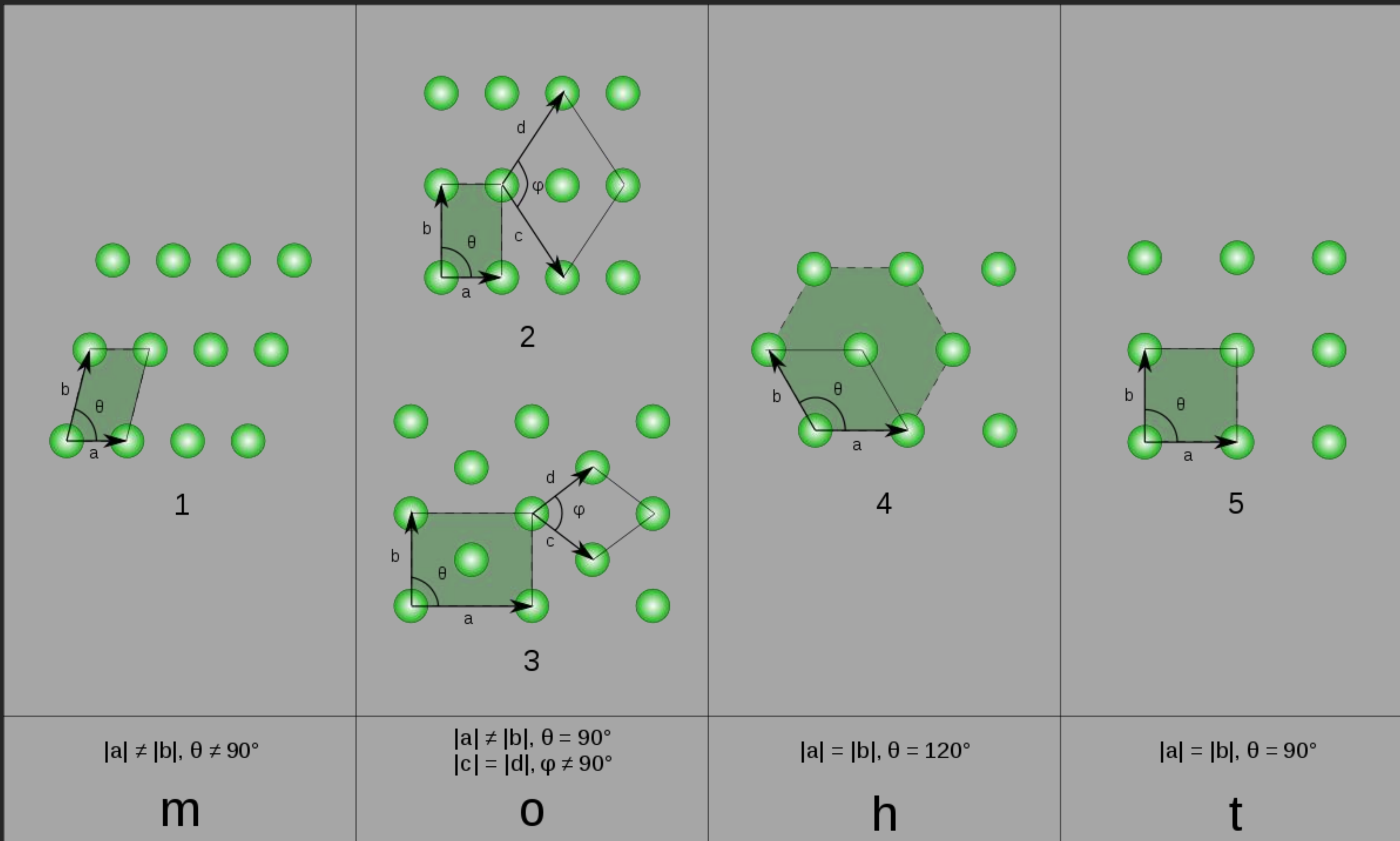
# What is a Bravais lattice?

**A Bravais lattice is an infinite array of discrete points generated by a set of discrete translation operations.**

**In planes, there are 5 Bravais lattices:**

- Oblique **2** (**m** = monoclinic)
- Rectangular **222** (**o** = orthorhombic)
  Centered rectangular **222** (**o** = orthorhombic)
- Hexagonal **622** (**h** = hexagonal)
- Square **422** (**t** = tetragonal)

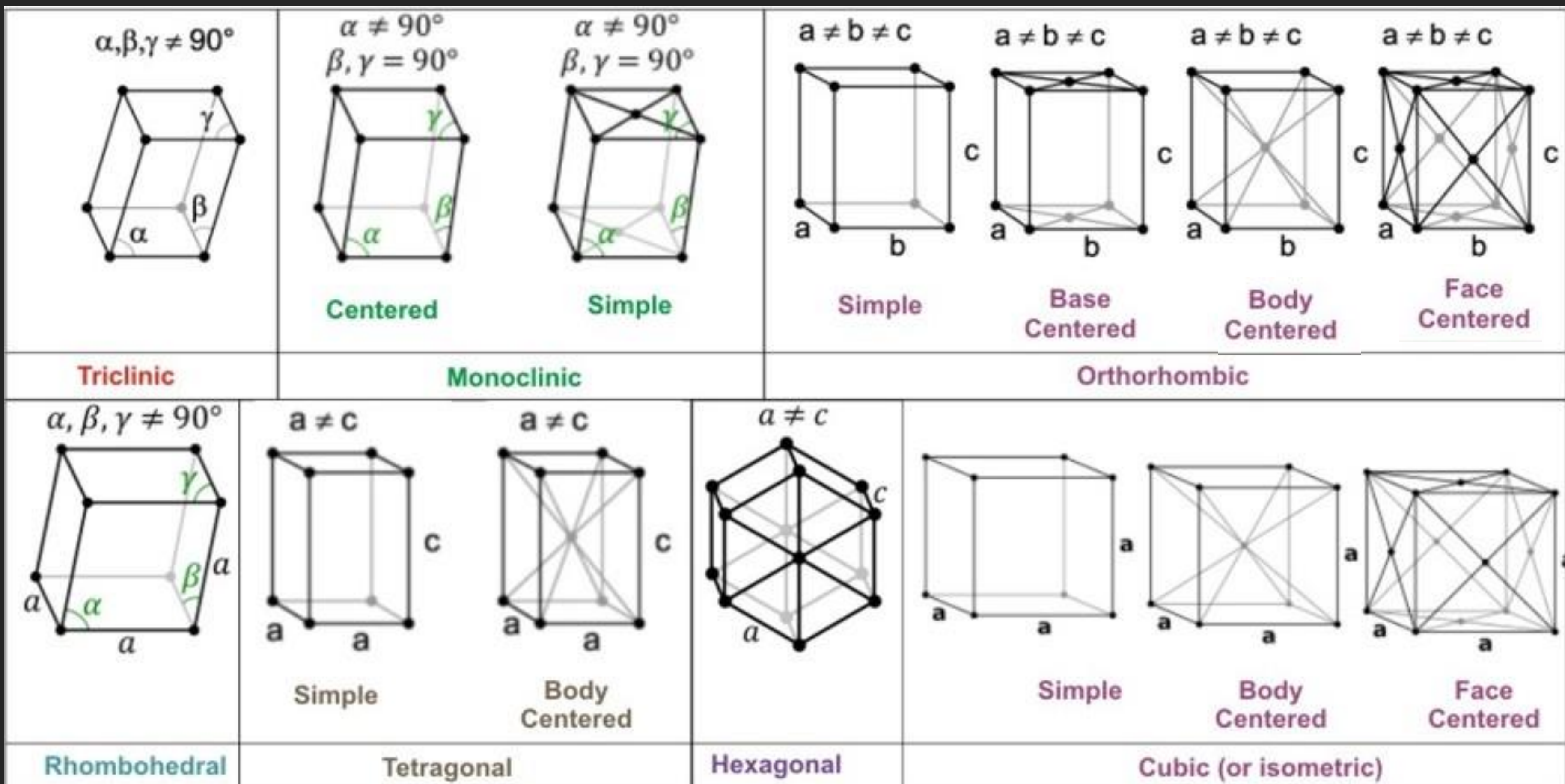
# What is a Bravais lattice?




Picture by Prolineserver

# In 3D:

…there are 14 Bravais lattices:




Picture from https://www.toppr.com/guides/chemistry/the-solid-state/space-lattice-or-crystal-lattice-and-unit-cell

# WARNING!

**THE SYMMETRY CONSTRAINS THE UNIT CELL…**

*For example: If you have a tetragonal symmetry (422), your unit cell needs to have $\alpha=\beta=\gamma=90°$ and $a=b$.*

**…NOT THE OTHER WAY ROUND!**

*You can have a unit cell with no symmetry and $\alpha=\beta=\gamma=90°$ and $a=b$, albeit unlikely.*

How to look it up

# READ THE INTERNATIONAL TABLES

# International tables

INTERNATIONAL TABLES
FOR
CRYSTALLOGRAPHY

*Volume A*
SPACE-GROUP SYMMETRY

*Edited by*
MOIS I. AROYO

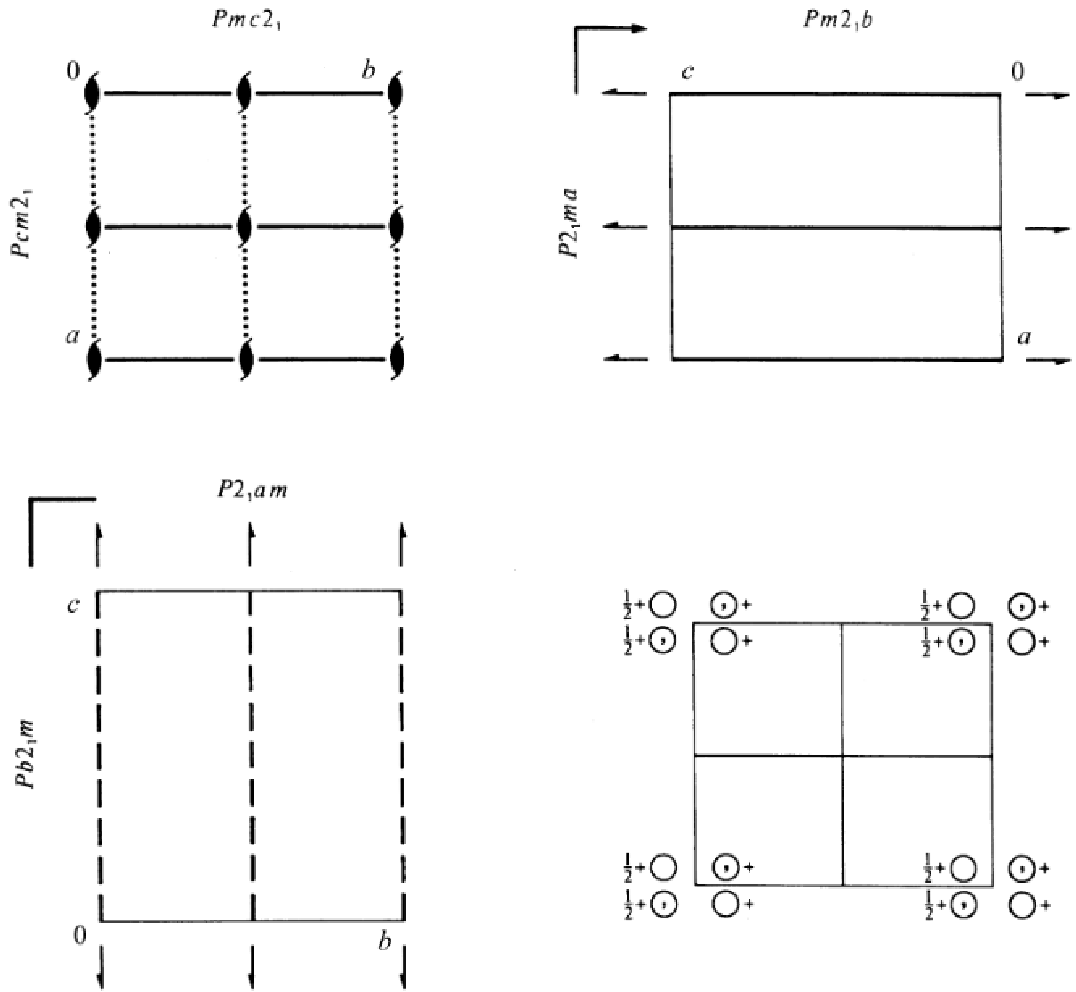
Sixth Edition

*Published for*
THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY

Dauter, Z. & Jaskolski M. (2010) J. Appl. Cryst. 43, 1150–1171
"How to read (and understand) Volume A of International Tables for Crystallography: an introduction for nonspecialists"

Orthorhombic $mm2$ $C_{2v}^{2}$ $Pmc2_1$

Patterson symmetry $Pmmm$ $Pmc2_1$ No. 26




**Origin** on $mc2_1$

http://img.chem.ucl.ac.uk/sgp/large/026az1.htm

**Origin** on $mc2_1$

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

**Symmetry operations**

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $c$ $x,0,z$ (4) $m$ $0,y,z$

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

**Positions**

| Multiplicity, Wyckoff letter, Site symmetry | | | Coordinates | | | | Reflection conditions |
|---|---|---|---|---|---|---|---|
| | | | | | | | General: |
| 4 | $c$ | 1 | (1) $x,y,z$ | (2) $\bar{x},\bar{y},z+\frac{1}{2}$ | (3) $x,\bar{y},z+\frac{1}{2}$ | (4) $\bar{x},y,z$ | $h0l$: $l=2n$<br>$00l$: $l=2n$ ? |
| | | | | | | | Special: no extra conditions |
| 2 | $b$ | $m\,.\,.$ | $\frac{1}{2},y,z$ | $\frac{1}{2},\bar{y},z+\frac{1}{2}$ | | | |
| 2 | $a$ | $m\,.\,.$ | $0,y,z$ | $0,\bar{y},z+\frac{1}{2}$ | | | |

**Symmetry of special projections**

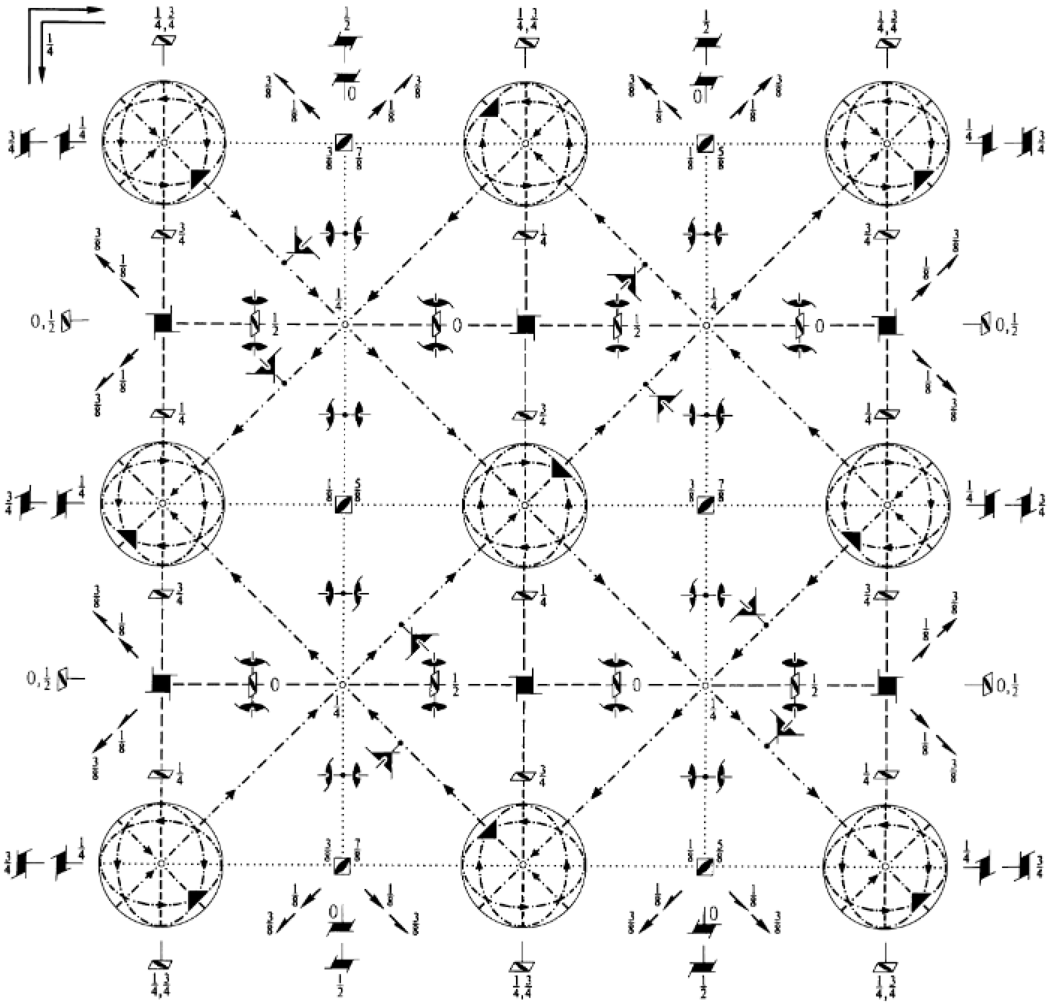
Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

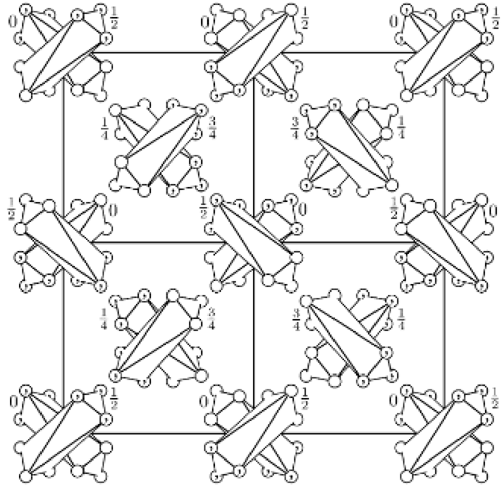
Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

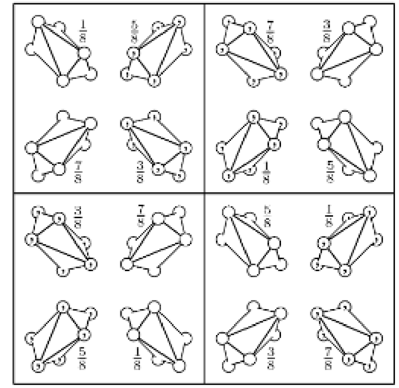
$Ia\bar{3}d$ $O_h^{10}$ $m\bar{3}m$ Cubic

No. 230 $I\ 4_1/a\ \bar{3}\ 2/d$ Patterson symmetry $Im\bar{3}m$





Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$

**Origin** at centre ($\bar{3}$)

**Asymmetric unit** $-\frac{1}{8}\le x\le\frac{1}{8};\quad -\frac{1}{8}\le y\le\frac{1}{8};\quad 0\le z\le\frac{1}{4};\quad \max(x,-x,y,-y)\le z$

Vertices $0,0,0\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}\quad -\frac{1}{8},\frac{1}{8},\frac{1}{8}\quad -\frac{1}{8},-\frac{1}{8},\frac{1}{8}\quad \frac{1}{8},-\frac{1}{8},\frac{1}{8}$

$\frac{1}{8},\frac{1}{8},\frac{1}{4}\quad -\frac{1}{8},\frac{1}{8},\frac{1}{4}\quad -\frac{1}{8},-\frac{1}{8},\frac{1}{4}\quad \frac{1}{8},-\frac{1}{8},\frac{1}{4}$

**Symmetry operations**

For (0,0,0)+ set

| | | | |
|---|---|---|---|
| (1) $1$ | (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},0,z$ | (3) $2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$ | (4) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$ |
| (5) $3^+\ x,x,x$ | (6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$ | (7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ | (8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$ |
| (9) $3^-\ x,x,x$ | (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x-\frac{1}{4},\frac{1}{8}$ | (14) $2\ x,\bar{x}+\frac{3}{4},\frac{3}{8}$ | (15) $4^-(0,0,\frac{3}{4})\ \frac{1}{4},0,z$ | (16) $4^+(0,0,\frac{1}{4})\ -\frac{1}{4},\frac{1}{2},z$ |
| (17) $4^-(\frac{3}{4},0,0)\ x,\frac{1}{4},0$ | (18) $2(0,\frac{1}{2},\frac{1}{2})\ \frac{1}{8},y+\frac{1}{4},y$ | (19) $2\ \frac{3}{8},y+\frac{3}{4},\bar{y}$ | (20) $4^+(\frac{1}{4},0,0)\ x,-\frac{1}{4},\frac{1}{2}$ |
| (21) $4^+(0,\frac{1}{4},0)\ \frac{1}{2},y,-\frac{1}{4}$ | (22) $2(\frac{1}{2},0,\frac{1}{2})\ x-\frac{1}{4},\frac{1}{8},x$ | (23) $4^-(0,\frac{3}{4},0)\ 0,y,\frac{1}{4}$ | (24) $2\ \bar{x}+\frac{3}{4},\frac{3}{8},x$ |
| (25) $\bar{1}\ 0,0,0$ | (26) $a\ x,y,\frac{1}{4}$ | (27) $c\ x,\frac{1}{4},z$ | (28) $b\ \frac{1}{4},y,z$ |
| (29) $\bar{3}^+\ x,x,x;\ 0,0,0$ | (30) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$ | (31) $\bar{3}^+\ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$ | (32) $\bar{3}^+\ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$ |
| (33) $\bar{3}^-\ x,x,x;\ 0,0,0$ | (34) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$ | (35) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$ | (36) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$ |
| (37) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})\ x+\frac{1}{2},\bar{x},z$ | (38) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ x,x,z$ | (39) $\bar{4}^-\ 0,\frac{3}{4},z;\ 0,\frac{3}{4},\frac{3}{8}$ | (40) $\bar{4}^+\ \frac{1}{2},-\frac{1}{4},z;\ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ |
| (41) $\bar{4}^-\ x,0,\frac{3}{4};\ \frac{1}{8},0,\frac{3}{4}$ | (42) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4})\ x,y+\frac{1}{2},\bar{y}$ | (43) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ x,y,y$ | (44) $\bar{4}^+\ x,\frac{1}{2},-\frac{1}{4};\ \frac{3}{8},\frac{1}{2},-\frac{1}{4}$ |
| (45) $\bar{4}^+\ -\frac{1}{4},y,\frac{1}{2};\ -\frac{1}{4},\frac{3}{8},\frac{1}{2}$ | (46) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4})\ \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^-\ \frac{3}{4},y,0;\ \frac{3}{4},\frac{1}{8},0$ | (48) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})\ x,y,x$ |

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

| | | | |
|---|---|---|---|
| (1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ | (2) $2\ 0,\frac{1}{4},z$ | (3) $2\ \frac{1}{4},y,0$ | (4) $2\ x,0,\frac{1}{4}$ |
| (5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ x,x,x$ | (6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ | (7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ |
| (9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ x,x,x$ | (10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ | (11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ | (12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ |
| (13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x+\frac{1}{4},\frac{3}{8}$ | (14) $2\ x,\bar{x}+\frac{1}{4},\frac{1}{8}$ | (15) $4^-(0,0,\frac{1}{4})\ \frac{3}{4},0,z$ | (16) $4^+(0,0,\frac{3}{4})\ \frac{1}{4},\frac{1}{2},z$ |
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| (21) $4^+(0,\frac{3}{4},0)\ \frac{1}{2},y,\frac{1}{4}$ | (22) $2(\frac{1}{2},0,\frac{1}{2})\ x+\frac{1}{4},\frac{3}{8},x$ | (23) $4^-(0,\frac{1}{4},0)\ 0,y,\frac{3}{4}$ | (24) $2\ \bar{x}+\frac{1}{4},\frac{1}{8},x$ |
| (25) $\bar{1}\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (26) $b\ x,y,0$ | (27) $a\ x,0,z$ | (28) $c\ 0,y,z$ |
| (29) $\bar{3}^+\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (30) $\bar{3}^+\ \bar{x}-\frac{1}{2},x,\bar{x};\ -\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (31) $\bar{3}^+\ x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ -\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ | (32) $\bar{3}^+\ \bar{x},\bar{x}-\frac{1}{2},x;\ \frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ |
| (33) $\bar{3}^-\ x,x,x;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (34) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$ | (35) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$ | (36) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$ |
| (37) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})\ x+\frac{1}{2},\bar{x},z$ | (38) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ x,x,z$ | (39) $\bar{4}^-\ 0,\frac{1}{4},z;\ 0,\frac{1}{4},\frac{3}{8}$ | (40) $\bar{4}^+\ \frac{1}{2},\frac{1}{4},z;\ \frac{1}{2},\frac{1}{4},\frac{1}{8}$ |
| (41) $\bar{4}^-\ x,0,\frac{1}{4};\ \frac{3}{8},0,\frac{1}{4}$ | (42) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4})\ x,y+\frac{1}{2},\bar{y}$ | (43) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ x,y,y$ | (44) $\bar{4}^+\ x,\frac{1}{2},\frac{1}{4};\ \frac{1}{8},\frac{1}{2},\frac{1}{4}$ |
| (45) $\bar{4}^+\ \frac{1}{4},y,\frac{1}{2};\ \frac{1}{4},\frac{1}{8},\frac{1}{2}$ | (46) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})\ \bar{x}+\frac{1}{2},y,x$ | (47) $\bar{4}^-\ \frac{1}{4},y,0;\ \frac{1}{4},\frac{3}{8},0$ | (48) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})\ x,y,x$ |

**Generators selected** (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

**Positions**

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$

$h,k,l$ permutable

General:

**96 h 1**

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

Reflection conditions (general):
$hkl$: $h+k+l=2n$
$0kl$: $k,l=2n$
$hhl$: $2h+l=4n$
$h00$: $h=4n$

Special: as above, plus

**48 g ..2**

| | | | |
|---|---|---|---|
| $\frac{1}{8},y,\bar{y}+\frac{1}{4}$ | $\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$ | $\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$ | $\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$ |
| $\bar{y}+\frac{1}{4},\frac{1}{8},y$ | $\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$ | $y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$ | $y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$ |
| $y,\bar{y}+\frac{1}{4},\frac{1}{8}$ | $\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$ | $y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$ | $\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$ |
| $\frac{7}{8},\bar{y},y+\frac{3}{4}$ | $\frac{5}{8},y,y+\frac{1}{4}$ | $\frac{1}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$ | $\frac{3}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$ |
| $y+\frac{3}{4},\frac{7}{8},\bar{y}$ | $y+\frac{1}{4},\frac{5}{8},y$ | $\bar{y}+\frac{3}{4},\frac{1}{8},\bar{y}+\frac{1}{2}$ | $\bar{y}+\frac{1}{4},\frac{3}{8},y+\frac{1}{2}$ |
| $\bar{y},y+\frac{3}{4},\frac{7}{8}$ | $y,y+\frac{1}{4},\frac{5}{8}$ | $\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{8}$ | $y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{8}$ |

$hkl$: $h=2n+1$ or $h=4n$

**48 f 2..**

| | | | | | |
|---|---|---|---|---|---|
| $x,0,\frac{1}{4}$ | $\bar{x}+\frac{1}{2},0,\frac{3}{4}$ | $\frac{1}{4},x,0$ | $\frac{3}{4},\bar{x}+\frac{1}{2},0$ | $0,\frac{1}{4},x$ | $0,\frac{3}{4},\bar{x}+\frac{1}{2}$ |
| $\frac{3}{4},x+\frac{1}{4},0$ | $\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$ | $x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$ | $\bar{x}+\frac{1}{4},0,\frac{1}{4}$ | $0,\frac{1}{4},\bar{x}+\frac{1}{4}$ | $\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$ |
| $\bar{x},0,\frac{3}{4}$ | $x+\frac{1}{2},0,\frac{1}{4}$ | $\frac{3}{4},\bar{x},0$ | $\frac{1}{4},x+\frac{1}{2},0$ | $0,\frac{3}{4},\bar{x}$ | $0,\frac{1}{4},x+\frac{1}{2}$ |
| $\frac{1}{4},\bar{x}+\frac{3}{4},0$ | $\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$ | $\bar{x}+\frac{1}{4},\frac{1}{2},\frac{3}{4}$ | $x+\frac{3}{4},0,\frac{3}{4}$ | $0,\frac{3}{4},x+\frac{3}{4}$ | $\frac{1}{2},\frac{3}{4},\bar{x}+\frac{1}{4}$ |

$hkl$: $2h+l=4n$

**32 e .3.**

| | | | |
|---|---|---|---|
| $x,x,x$ | $\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$ | $\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ | $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$ |
| $x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$ | $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$ | $x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$ | $\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$ |
| $\bar{x},\bar{x},\bar{x}$ | $x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$ | $x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$ | $\bar{x}+\frac{1}{2},x+\frac{1}{2},x$ |
| $\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$ | $x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$ | $\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$ | $x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$ |

$hkl$: $h=2n+1$ or $h+k+l=4n$

**24 d $\bar{4}$..**

| | | | | | |
|---|---|---|---|---|---|
| $\frac{3}{8},0,\frac{1}{4}$ | $\frac{1}{8},0,\frac{3}{4}$ | $\frac{1}{4},\frac{3}{8},0$ | $\frac{3}{4},\frac{1}{8},0$ | $0,\frac{1}{4},\frac{3}{8}$ | $0,\frac{3}{4},\frac{1}{8}$ |
| $\frac{3}{4},\frac{5}{8},0$ | $\frac{3}{4},\frac{3}{8},\frac{1}{2}$ | $\frac{1}{8},\frac{1}{2},\frac{1}{4}$ | $\frac{7}{8},0,\frac{1}{4}$ | $0,\frac{1}{4},\frac{7}{8}$ | $\frac{1}{2},\frac{1}{4},\frac{1}{8}$ |

**24 c 2.22**

| | | | | | |
|---|---|---|---|---|---|
| $\frac{1}{8},0,\frac{1}{4}$ | $\frac{3}{8},0,\frac{3}{4}$ | $\frac{1}{4},\frac{1}{8},0$ | $\frac{3}{4},\frac{3}{8},0$ | $0,\frac{1}{4},\frac{1}{8}$ | $0,\frac{3}{4},\frac{3}{8}$ |
| $\frac{7}{8},0,\frac{3}{4}$ | $\frac{5}{8},0,\frac{1}{4}$ | $\frac{3}{4},\frac{7}{8},0$ | $\frac{1}{4},\frac{5}{8},0$ | $0,\frac{3}{4},\frac{7}{8}$ | $0,\frac{1}{4},\frac{5}{8}$ |

(24 d and 24 c) $hkl$: $h,k=2n$, $h+k+l=4n$ or $h,k=2n+1$, $l=4n+2$ or $h=8n$, $k=8n+4$ and $h+k+l=4n+2$

**16 b .32**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ | $\frac{3}{8},\frac{7}{8},\frac{5}{8}$ | $\frac{7}{8},\frac{5}{8},\frac{3}{8}$ | $\frac{5}{8},\frac{3}{8},\frac{7}{8}$ | $\frac{7}{8},\frac{7}{8},\frac{7}{8}$ | $\frac{5}{8},\frac{1}{8},\frac{3}{8}$ | $\frac{1}{8},\frac{3}{8},\frac{5}{8}$ | $\frac{3}{8},\frac{5}{8},\frac{1}{8}$ |

$hkl$: $h,k=2n+1$, $l=4n+2$ or $h,k,l=4n$

**16 a .$\bar{3}$.**

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $0,0,0$ | $\frac{1}{2},0,\frac{1}{2}$ | $0,\frac{1}{2},\frac{1}{2}$ | $\frac{1}{2},\frac{1}{2},0$ | $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ | $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ | $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ | $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ |

$hkl$: $h,k=2n$, $h+k+l=4n$

# How can we know?

In practice

# LAUE GROUP & MISSING REFLECTIONS

# Laue geometry

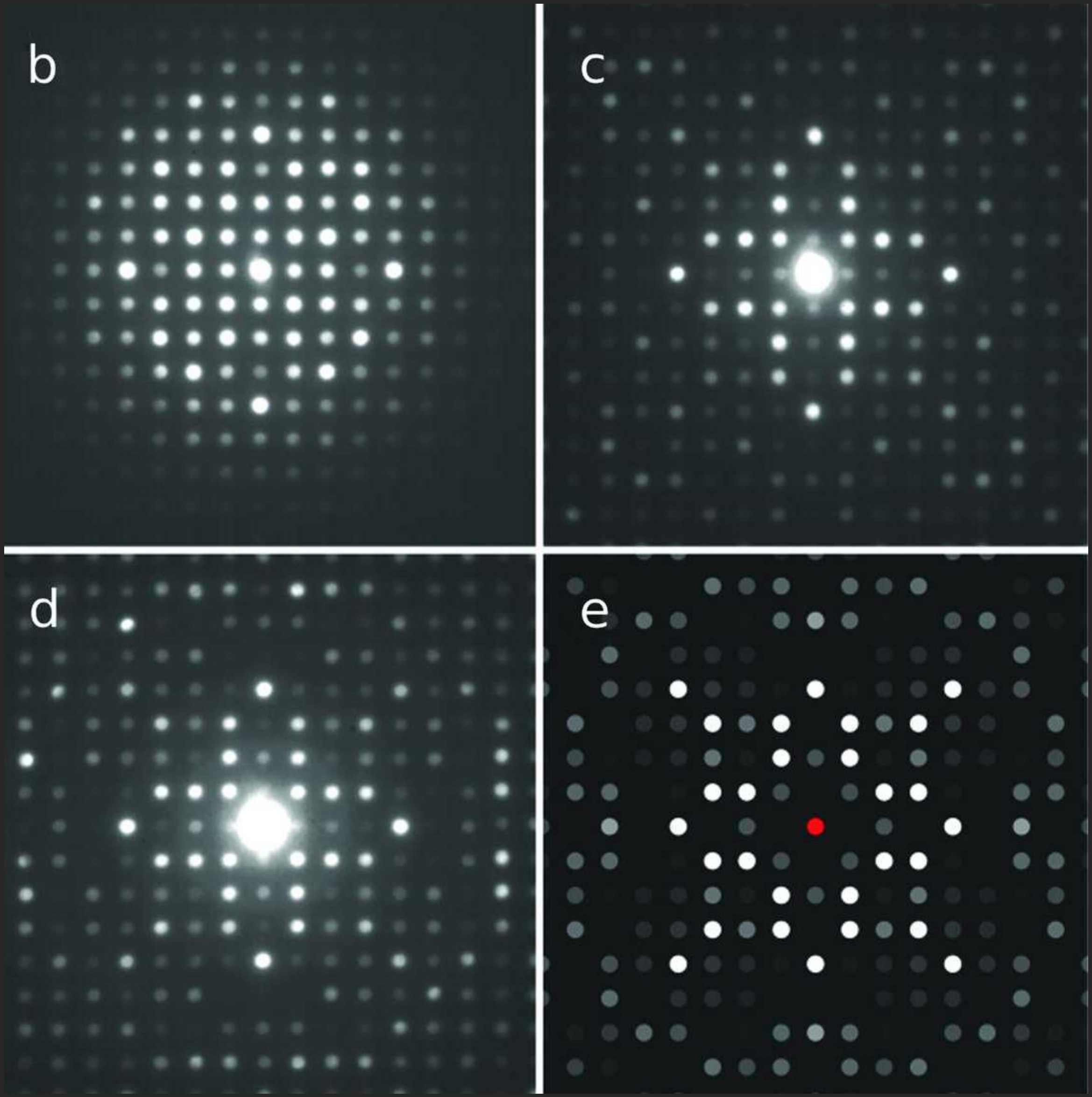
The shape of a crystal does not always reveal its symmetry as faces can grow at different rates.

The symmetry of the diffraction pattern reveals more.

For example: A fourfold symmetry axis in the diffraction must correspond to a 4, -4, $4_1$, $4_2$ or $4_3$ axis in the space group.

**Friedel's law:** Diffraction pattern is always centrosymmetric.

# Precession: Reciprocal space slices




From: Precession electron diffraction – a topical review, Midgleva, P.A. & Eggemana, A.S. (2015) IUCrJ 2, 126-136.

# Laue geometry

Crystals can belong to one of:

- 230 space groups
- 32 point groups

**but only 11 Laue groups:**

| | |
|---|---|
| -1 | -3 |
| 2/m | -3m |
| mmm | 6/m |
| 4/m | 6/mmm |
| 4/mmm | m3 |
| | m-3m |

# E-value statistics

- E-values are normalized structure factor amplitudes.

$$|E_{hkl}|^2 = \frac{|F_{hkl}|^2/\epsilon}{< |F_{hkl}|^2/\epsilon >}$$

$\varepsilon$ scale factor for proper treatment of special position reflections

$<|F_{hkl}|^2/\varepsilon>$ mean per resolution shell

- Centrosymmetric structures: E-values vary more.

$$< \left|E_{hkl}^2 - 1\right| >$$

**0.968** if the space group is centrosymmetric

**0.736** for non-centrosymmetric space groups

**Lower:** twinned crystal?

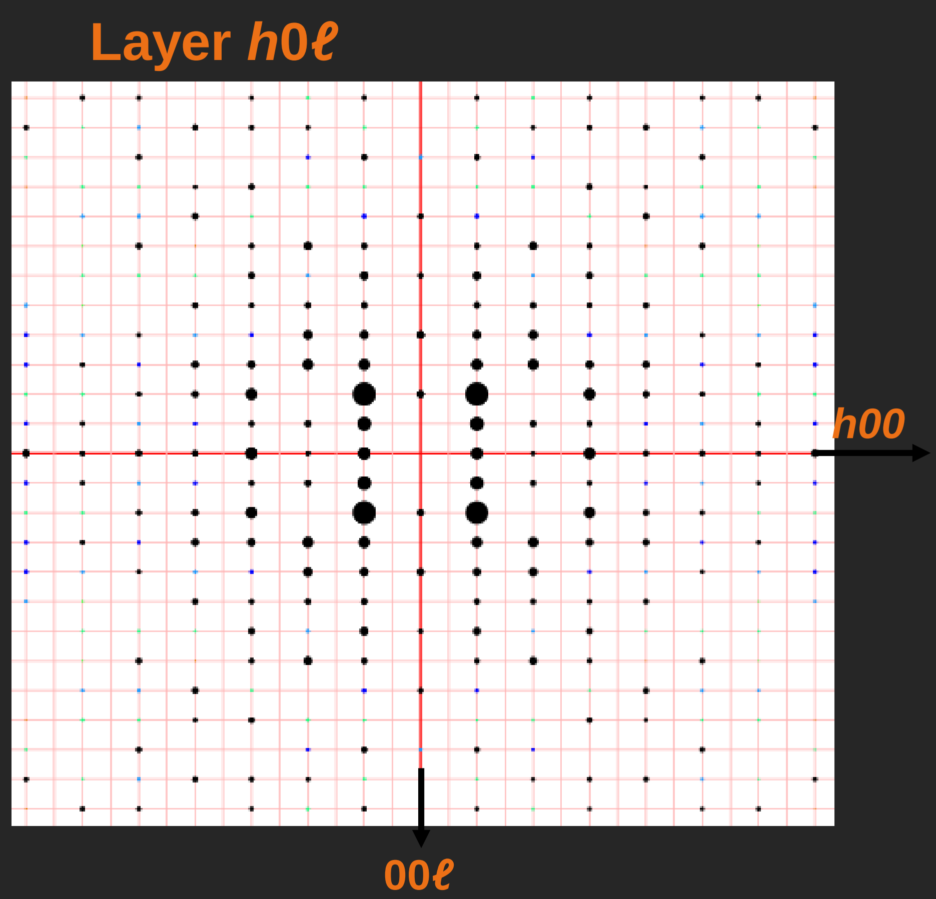
# But I want to know the space group!

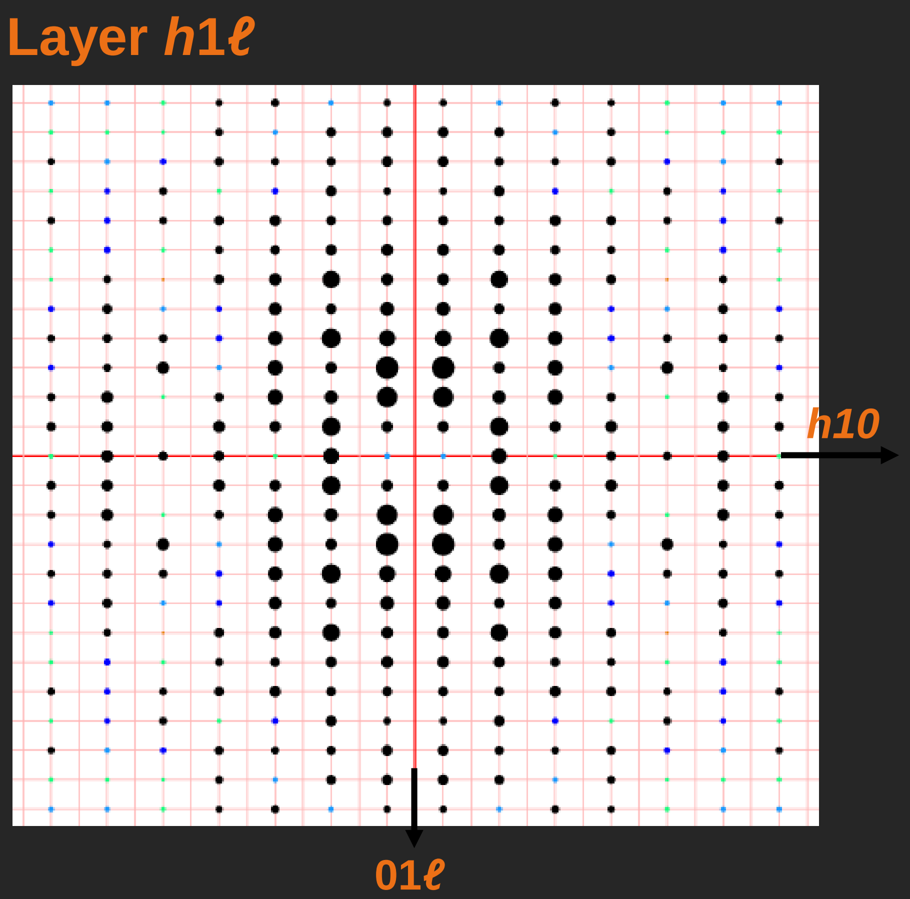
1) If you are a protein crystallographer, you only have to consider space groups without mirror planes, glides planes and inversion centres. (Why?)
   **Sohnke groups:** Only 65 of 230 space groups.
2) Are reflections systematically missing?
   Translational symmetry makes intensities become 0!

   **For example:**
   $2_1$ screw axis along a
   every second reflection h00 is absent

   **Reflection condition:** h00 =2n

# Systematic absences




Laue: mmm (orthorhombic)

Reflections *h+k≠2n* absent - lattice type C.

In addition, the reflections 00ℓ are absent when ℓ is odd - $2_1$ screw axis along c.

This fits only the space group $C222_1$!

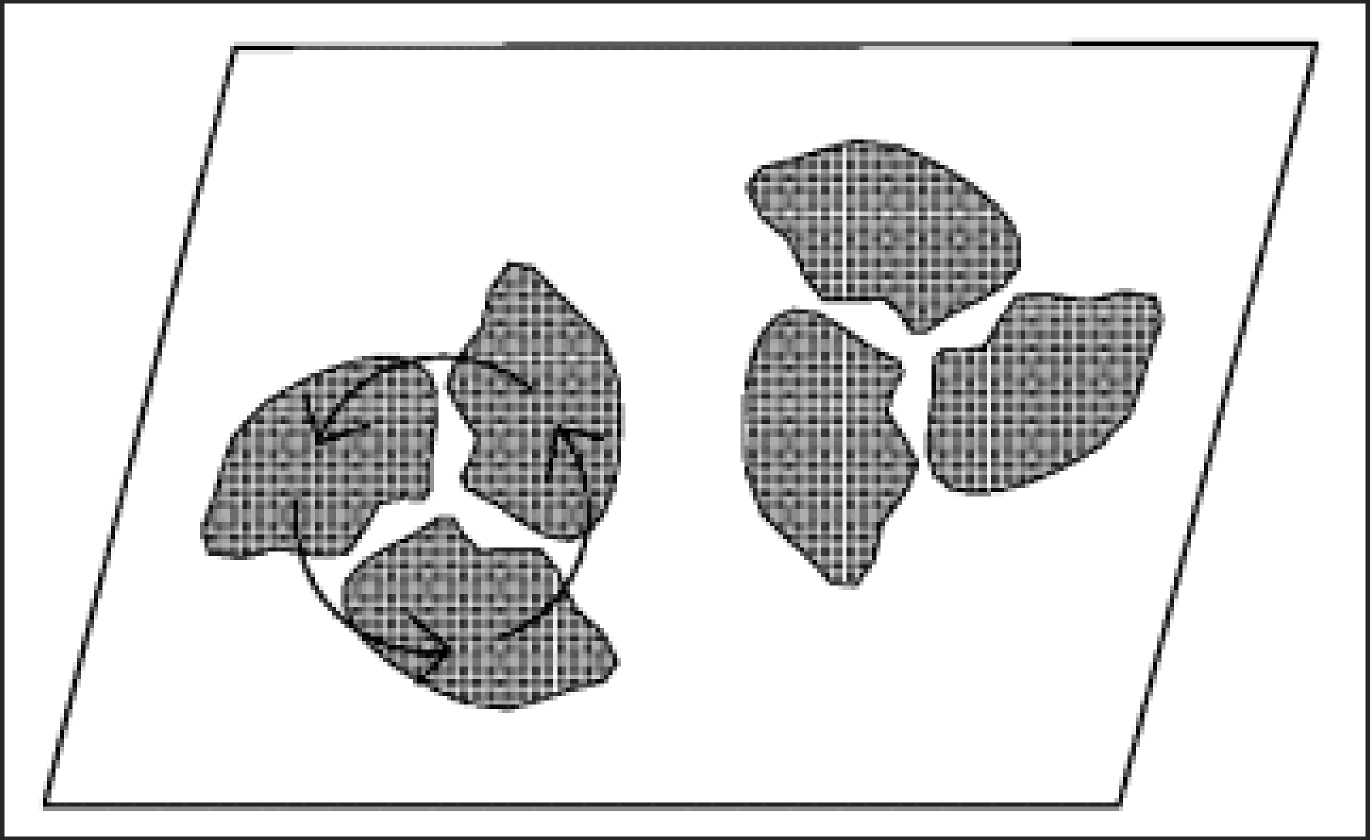
Pictures courtesy of George Sheldrick

Got more symmetry than you bargained for?

# NON-CRYSTALLOGRAPHIC SYMMETRY
# TWINNING

# What is non-crystallographic symmetry?

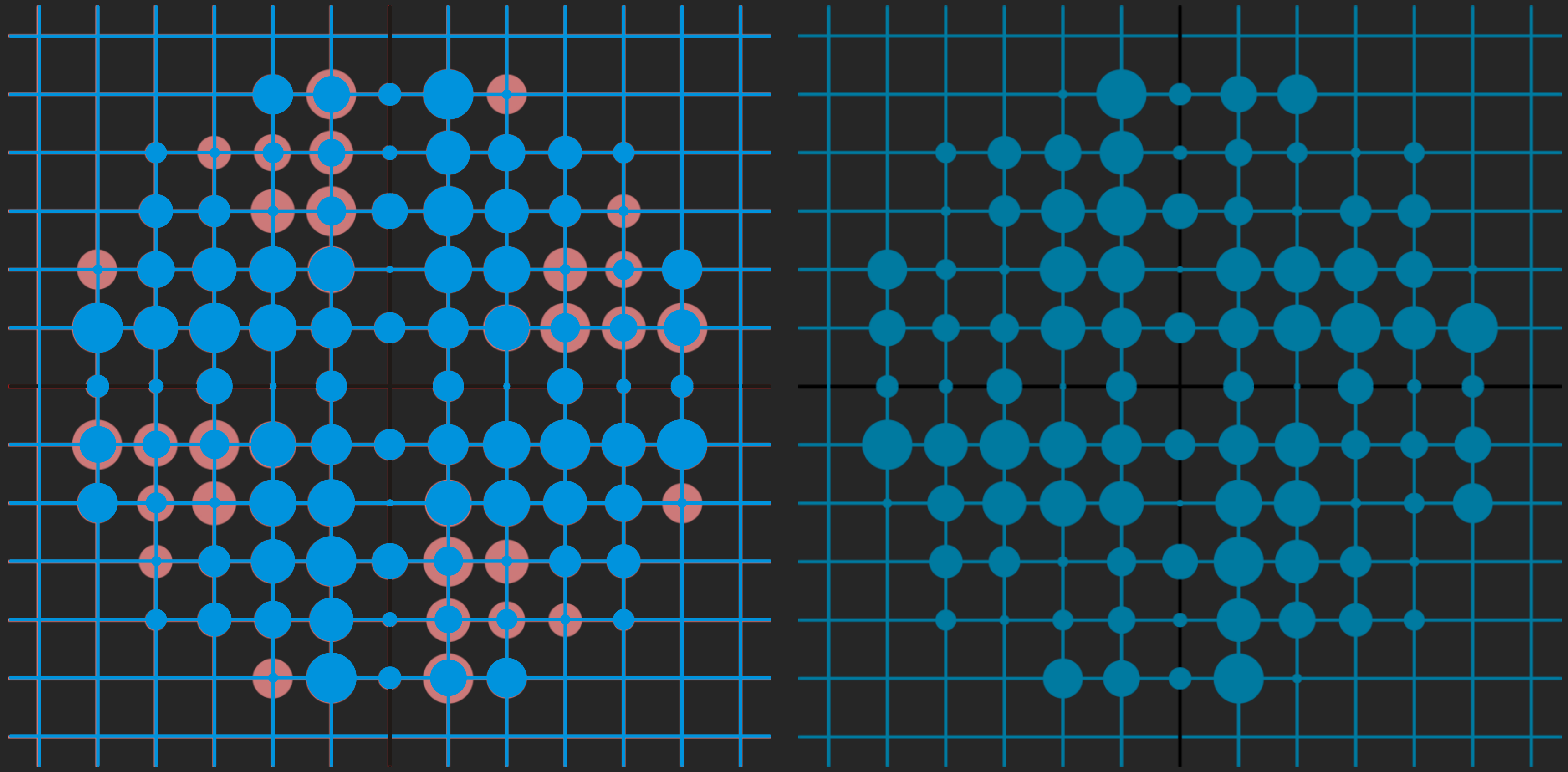
A symmetry operation that is not compatible with the periodicity of a crystal pattern.



Picture from CCP4Wiki: http://www.ysbl.york.ac.uk/~cowtan/ccp4wiki/wiki71.html

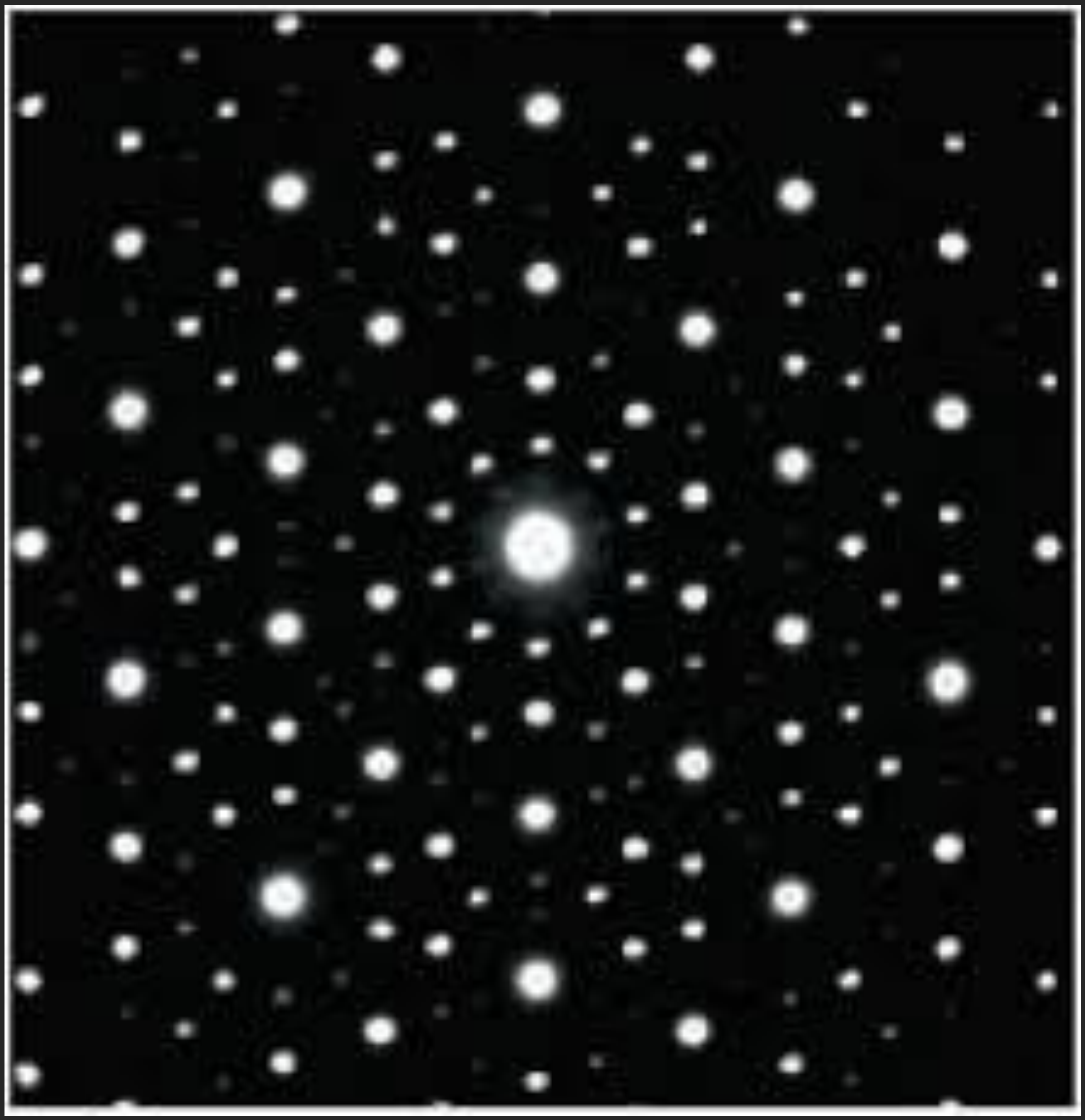
# Twinning

More than one crystal grown together in different orientation.

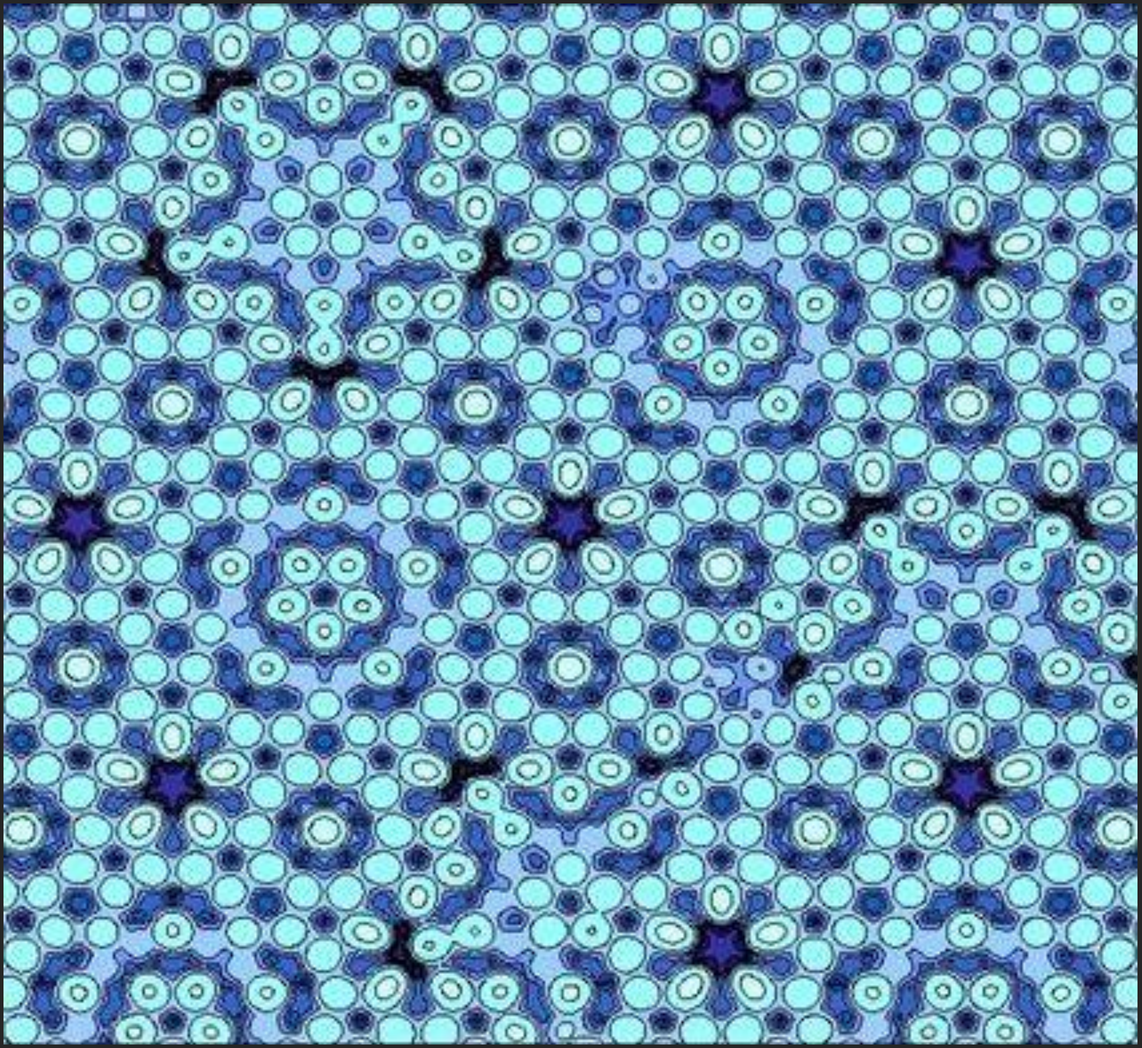


**Want to know more? Watch: https://www.youtube.com/watch?v=WF7j94sUi1w**

# What is the symmetry in this picture?



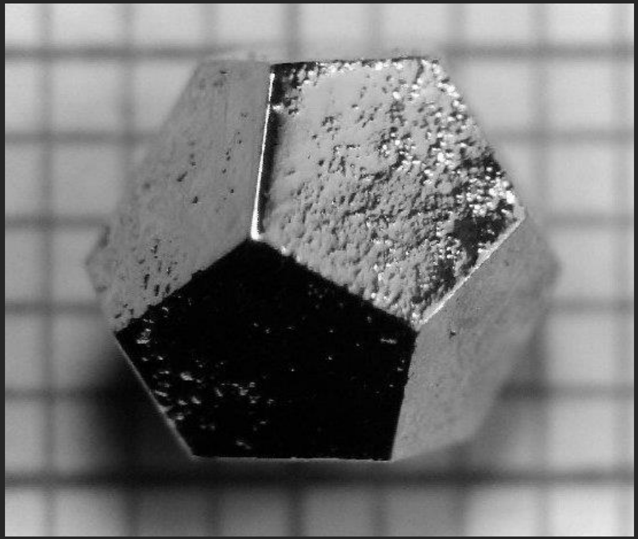
# Quasi crystals



Picture: J.W. Evans, The Ames Laboratory, US Department of Energ

# Definition: Crystal

A material is a crystal if it has essentially a sharp diffraction pattern.



Picture: Ho-Mg-Zn dodecahedral quasicrystal, The Ames Laboratory, US Department of Energ

Full definition: https://dictionary.iucr.org/Crystal

# Summary

- **Point groups** give symmetry with no translation
- **Plane** and **space groups** include translation
- **Bravais lattices** are infinite arrays of points.
- **International Tables Vol. A** is where to look things up.
- **Diffraction** patterns belong to one of **11 Laue groups** (in 3D)
- Laue group, E value statistics and systematic absences allow us to **determine the space group** (or at least narrow things down.)
- **Non-crystallographic symmetry** and **twinning** also exist.