Space group determination

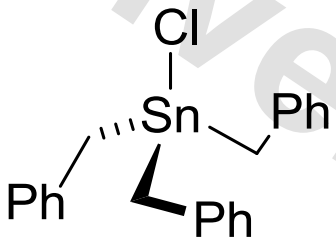
Some figures have been copied from slides of G. M. Sheldrick

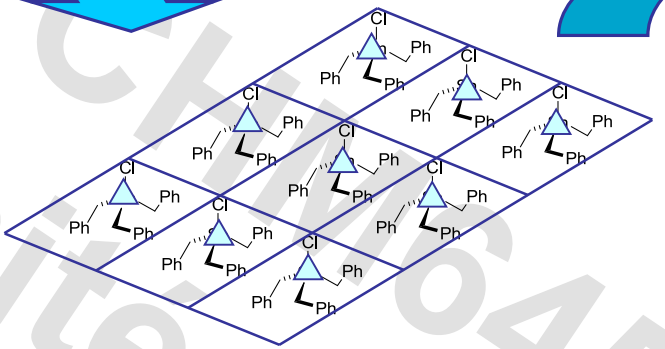
Internet sources to consult: (and lots of others)
http://img.chem.ucl.ac.uk/sgp/mainmenu.htm
http://subaru2.univ-lemans.fr/enseignements/physique/02/cristallo/bravais.html
http://subaru2.univ-lemans.fr/enseignements/physique/02/cristallo/espace.html

Structure determination

Crystallisation

Single crystal selection





***Molecular structure**:*
Atomic positions

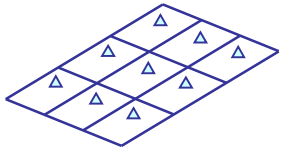
***Crystalline structure**:*
Unit cell and space group

***Crystal**:*
Macroscopic dimensions

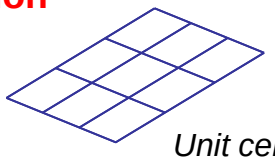
Solution and Refinement

Dataset collection

H	K	L	I	σ
0	0	1	134.4	12.5
0	0	2	0.2	1.2
1	1	4	52.4	2.2

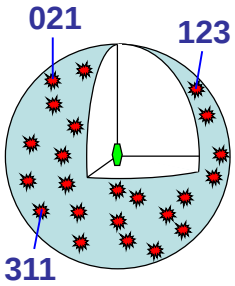


Space group determination

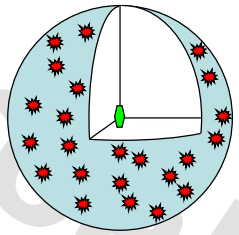


Unit cell

H	K	L	I	σ
0	0	1	134.4	12.5
0	0	2	0.2	1.2
1	1	4	52.4	2.2



Détermination of the unit cell



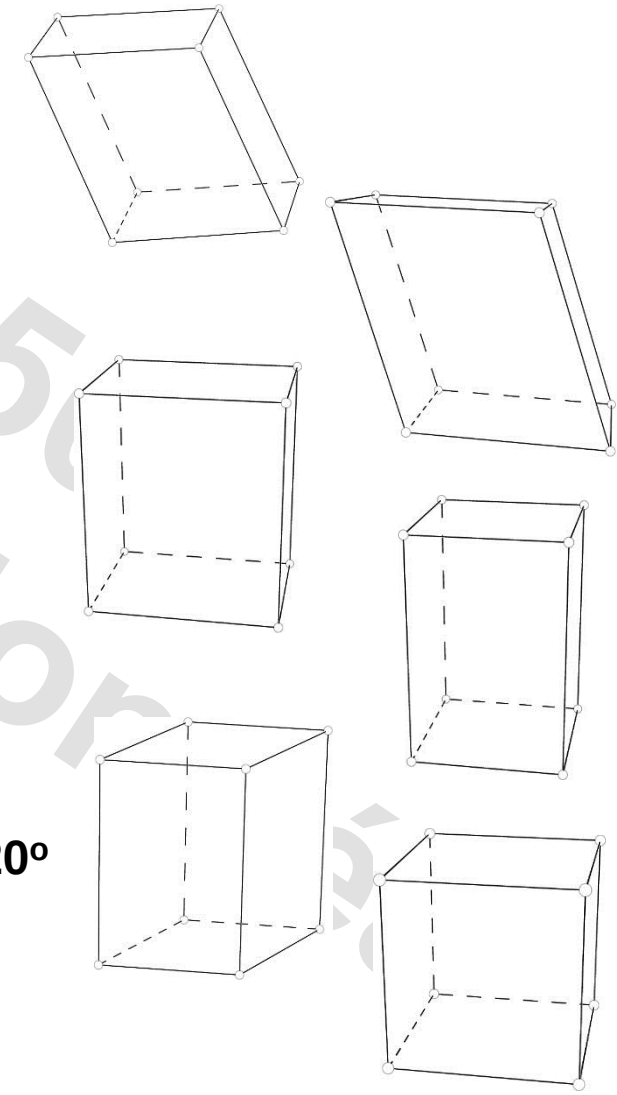
Raw data

***Unit cell + space group**:*
Dimensions and symmetry of the crystalline structure
Intensity of the reflections:
Atomic positions

The seven crystal systems

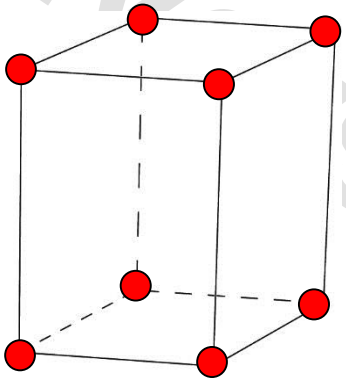
Which possibilities exist for a unit cell ?

	Dimension conditions	Angle conditions
Triclinic	-	-
Monoclinic	-	$\alpha = \gamma = 90^o$
Orthorhombic	-	$\alpha = \beta = \gamma = 90^o$
Tetragonal	$a = b$	$\alpha = \beta = \gamma = 90^o$
Trigonal, hexagonal	$a = b$	$\alpha = \beta = 90^o, \gamma = 120^o$
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^o$

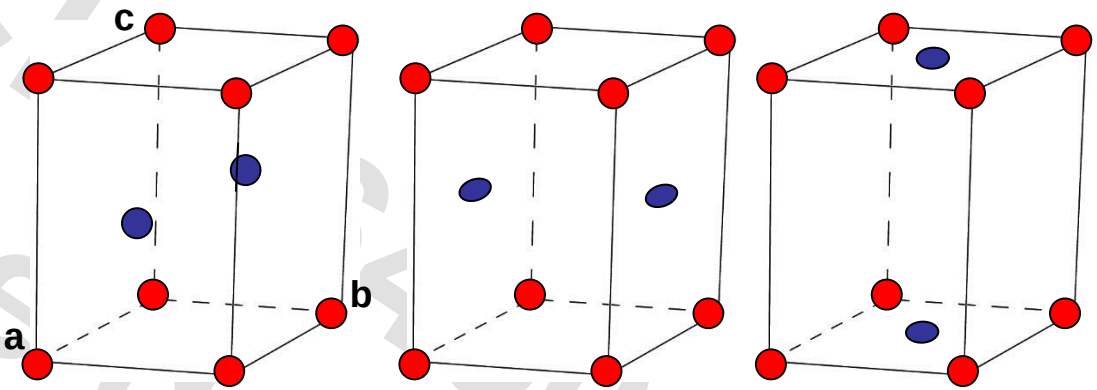


The 14 Bravais lattices

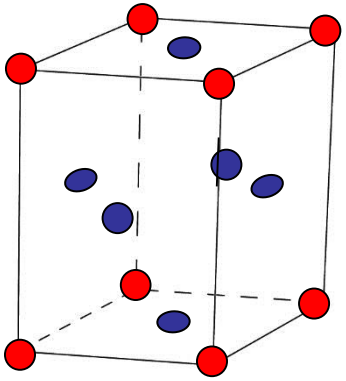
We obtain 14 Bravais lattices, when we combine the crystal systems with the centering. Centering describes that more than one “unit”/molecule is present in the unit cell (additional translational symmetry).



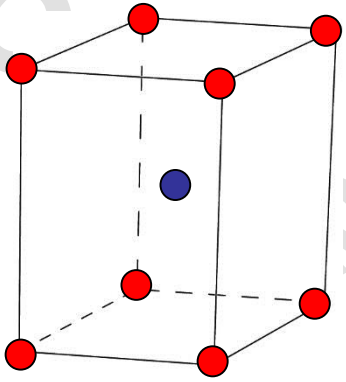
Primitive (*simple*) **P**



Face centered (*face centrée*) **A, B, C**

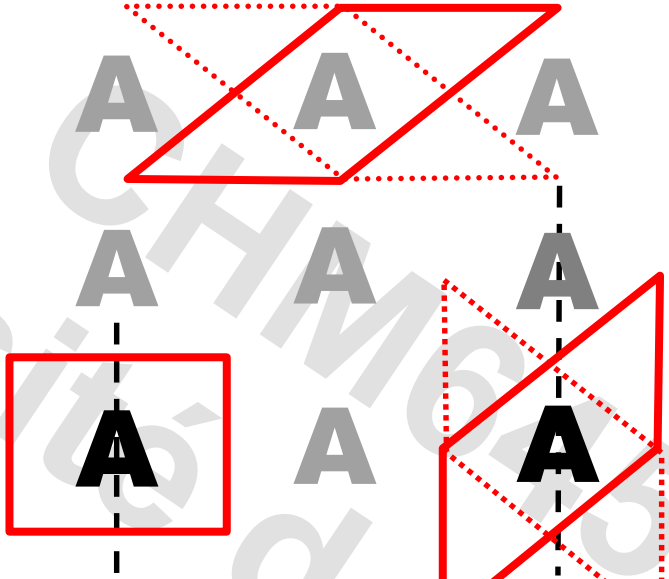


All-faces centered (*faces centrées*) **F**



Body centered (*centré*) **I**

Why do we need centered lattices ?

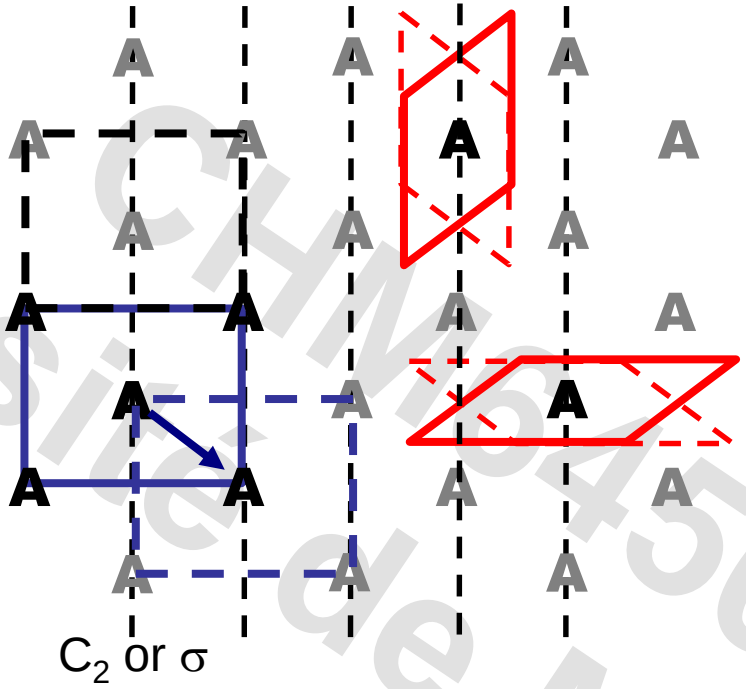


In the absence of symmetry, we can choose every possible unit cell.

If a C_2 rotation axis or a mirror plane is present, only a monoclinc unit cell (or higher) is compatible with these symmetry elements. Without that symmetry it wouldn't even be a monoclinic cell: it would be a triclinic cell with angles very, very close to 90°!

To correctly describe our structure, we have always to choose the highest possible symmetry.

Why do we need centered lattices ?

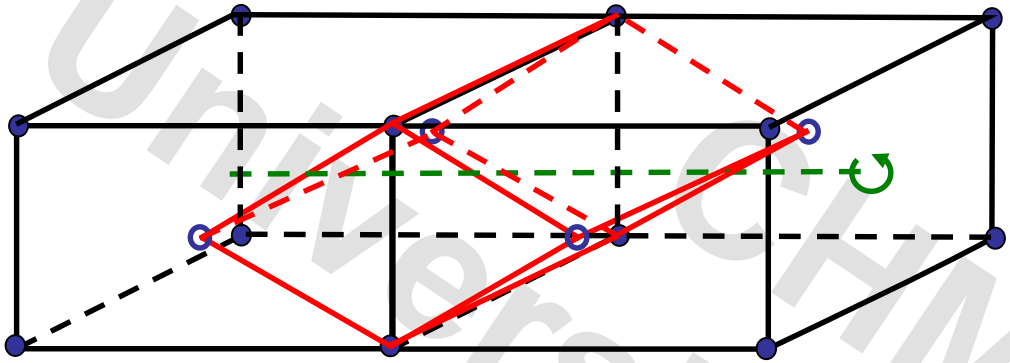


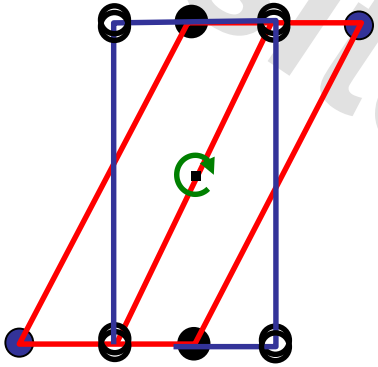
How can we describe a crystal which contains a certain symmetry, for example a C_2 axis or a mirror plane, but the smallest cells are incompatible with these symmetry elements.

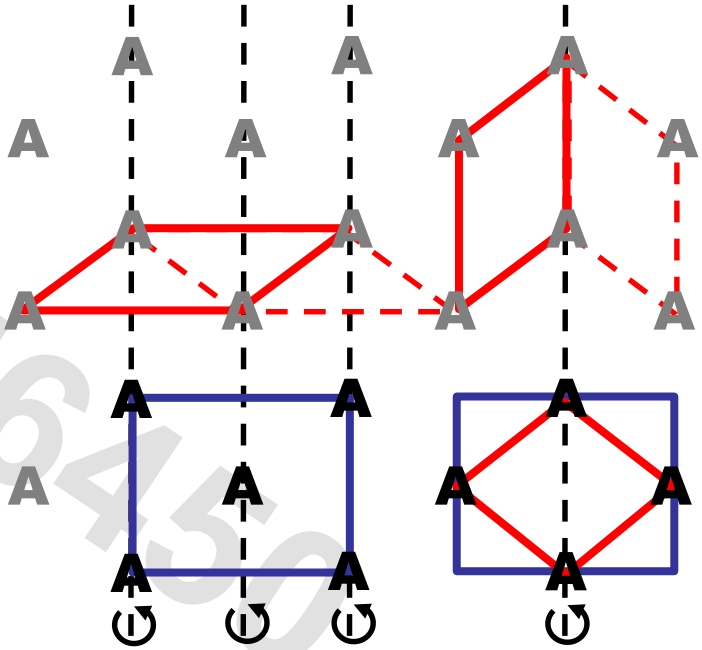
We choose a cell of higher volume, containing more than one lattice point, a so called centered cell. In this example, we have a centered monoclinic cell.

In crystallographic language, a face centering C adds to the existing translations (x+1,y,z; x,y+1,z; x,y,z+1) another one with x+0.5, y+0.5, z.

Actually… we do not need them!





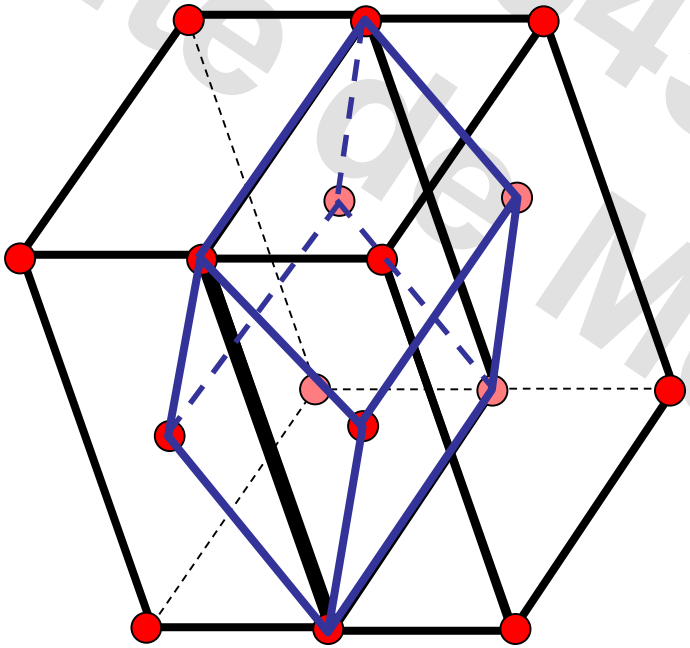


- There is a triclinic cell which is compatible with a C_2 axis or a mirror plane: triclinic with a = c and $\alpha = \gamma$.
- But instead of introducing additional unit cells, centering was introduced.
- Thus instead of 14 crystal systems, we have 7 crystal systems + centering = 14 Bravais lattices

The 14 Bravais lattices

7 crystal systems and 6 centerings: Why do we not have 42 Bravais lattices?

Triclinic: **Only P (primitive)**. Every centered lattice can be transformed into a primitive one.



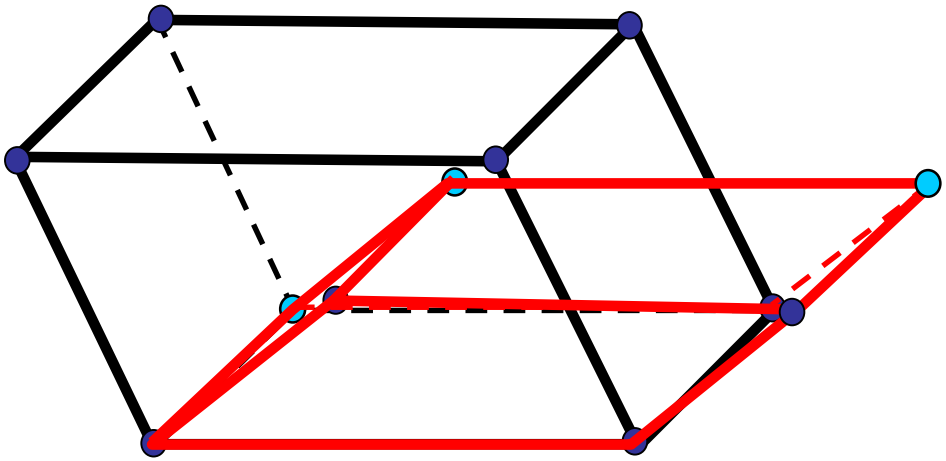
The 14 Bravais lattices

7 crystal systems and 6 centerings: Why do we not have 42 Bravais lattices?

Triclinic: **Only aP**

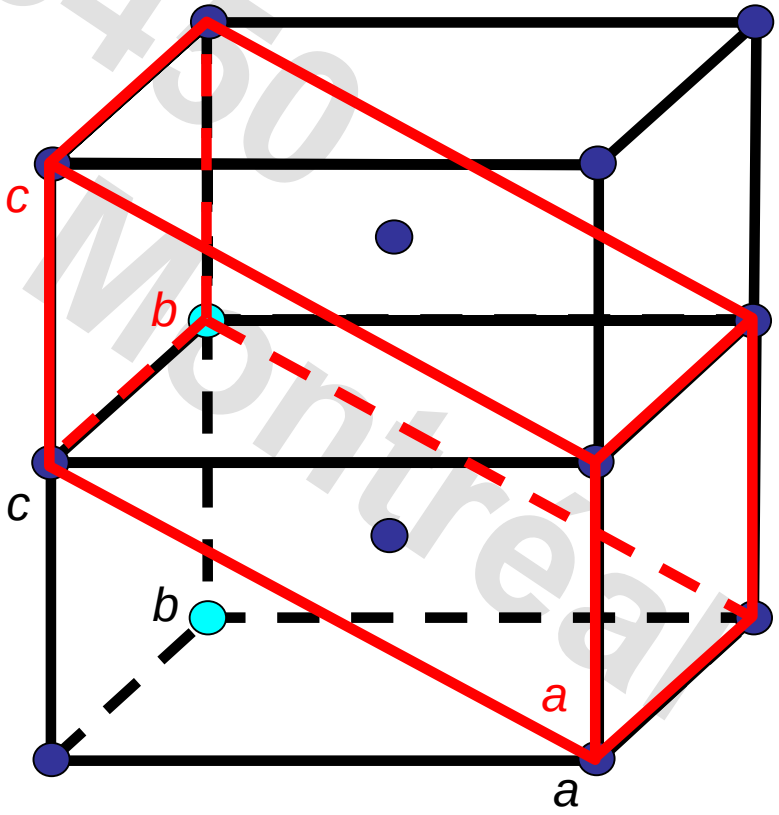
Monoclinic: Only mP and mC

- **A** can be transformed into **C** by exchanging the axes a and c.
- **B** can be transformed into **P**.
- **I** can be transformed into **C**.



mB → mP

mI → mC



The 14 Bravais lattices

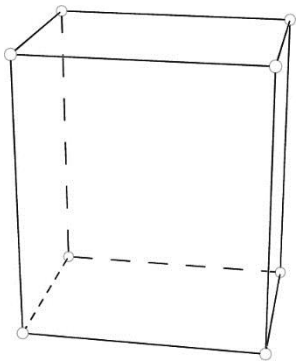
7 crystal systems and 6 centerings: Why do we not have 42 Bravais lattices?

Triclinic: **Only aP**

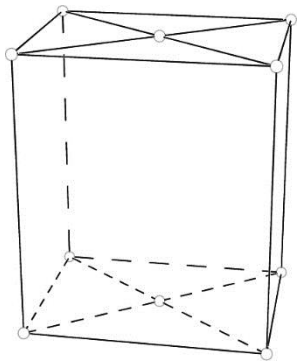
Monoclinic: Only mP and mC

Orthorhombic: oP, oA, oI, oF

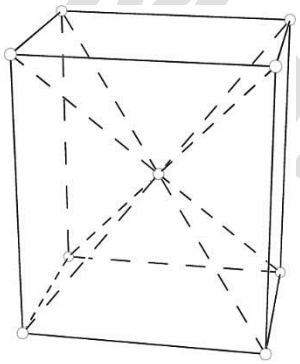
oB and **oC** can be transformed into **oA** by simple axis exchange



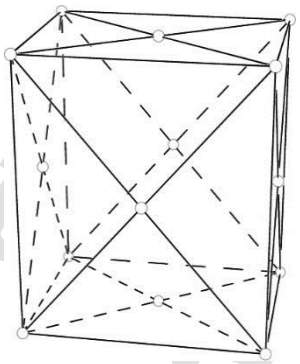
oP



oA



oI



oF

The 14 Bravais lattices

7 crystal systems and 6 centerings: Why do we not have 42 Bravais lattices?

Triclinic: **Only aP**

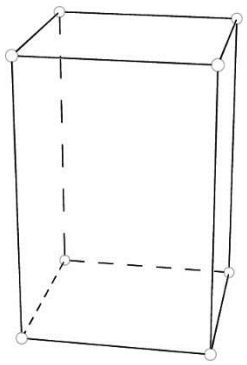
Monoclinic: Only mP and mC

Orthorhombic: oP, oA, oI, oF

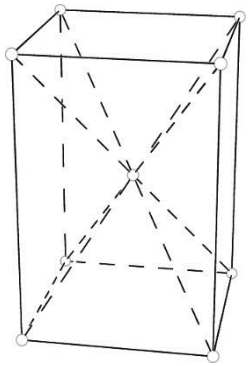
Tetragonal: tP and tI (Because of the C_4-symmetry, **tA** becomes **tF**, which can be transformed into **tI**. **tC** can be transformed into **tP**.)

Trigonal, hexagonal

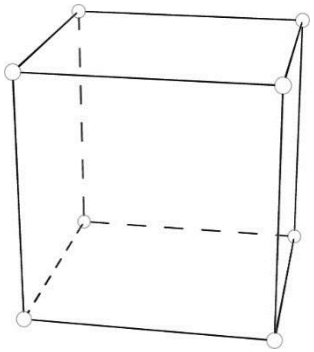
Cubique: cP, cI et cF (C_3 symmetry: **cA/cB/cC** become automatically **cF**)



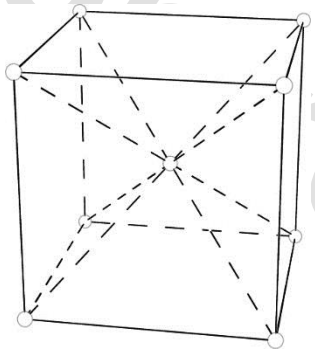
tP



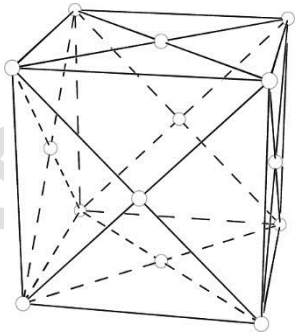
tI



cP



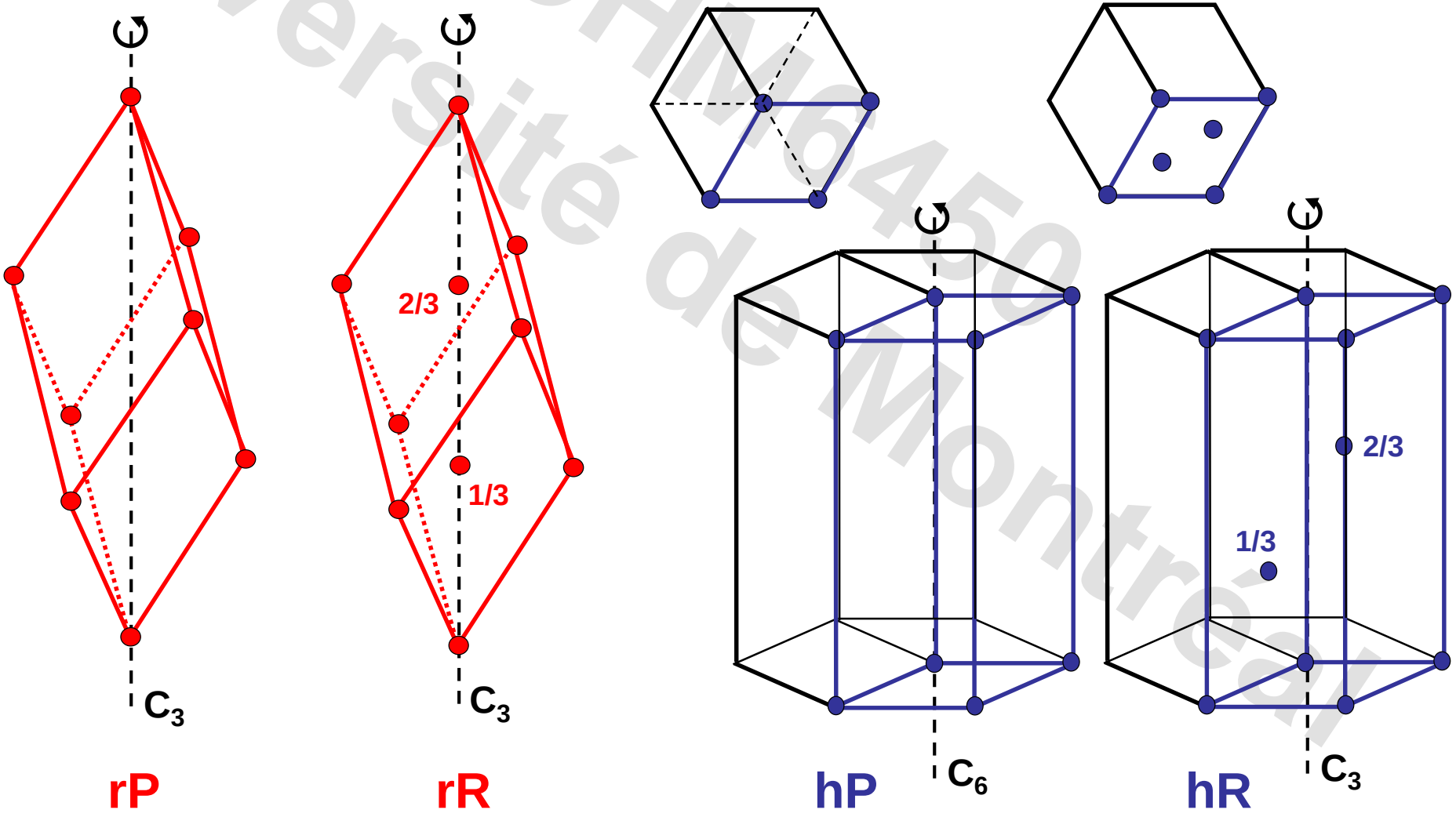
cI



cF

Trigonal, hexagonal, rhomboédrique

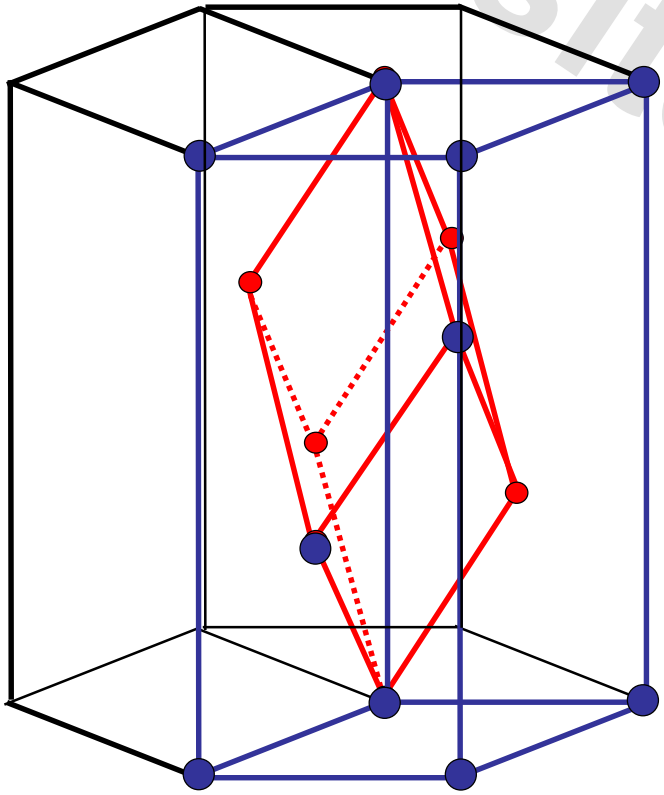
The trigonal/rhombohedral (a=b=c, $\alpha=\beta=\gamma\neq90^o$) and hexagonal (a=b, $\alpha=\beta=90^o$, $\gamma=120^o$) crystal systems can only have rhombohedral centering to be compatible with C_3 and C_6 symmetry.

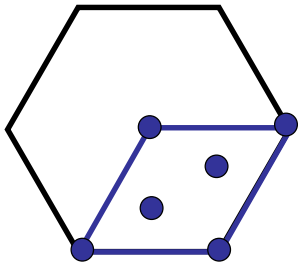


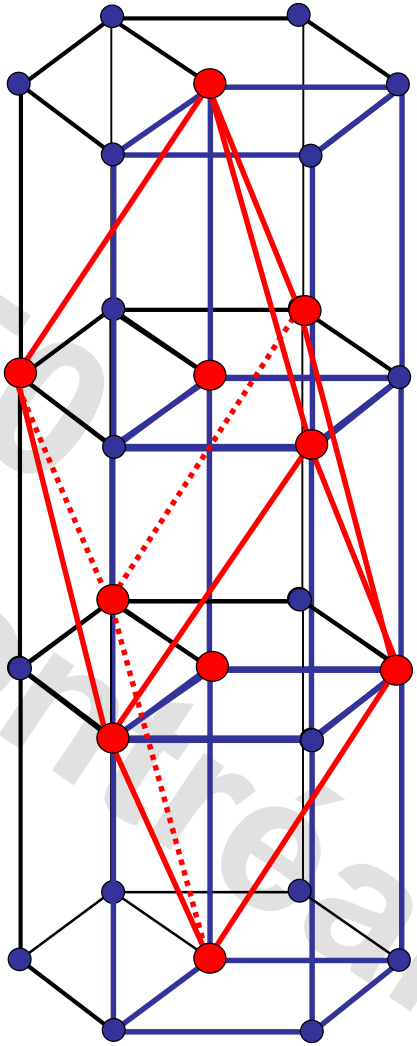
Transformation rhomboédrique - hexagonal

Rhombohedral (trigonal) primitive (**rP**) can be transformed into **hR**.

Hexagonal primivitive (**hP**) can be transformed into **rR**.

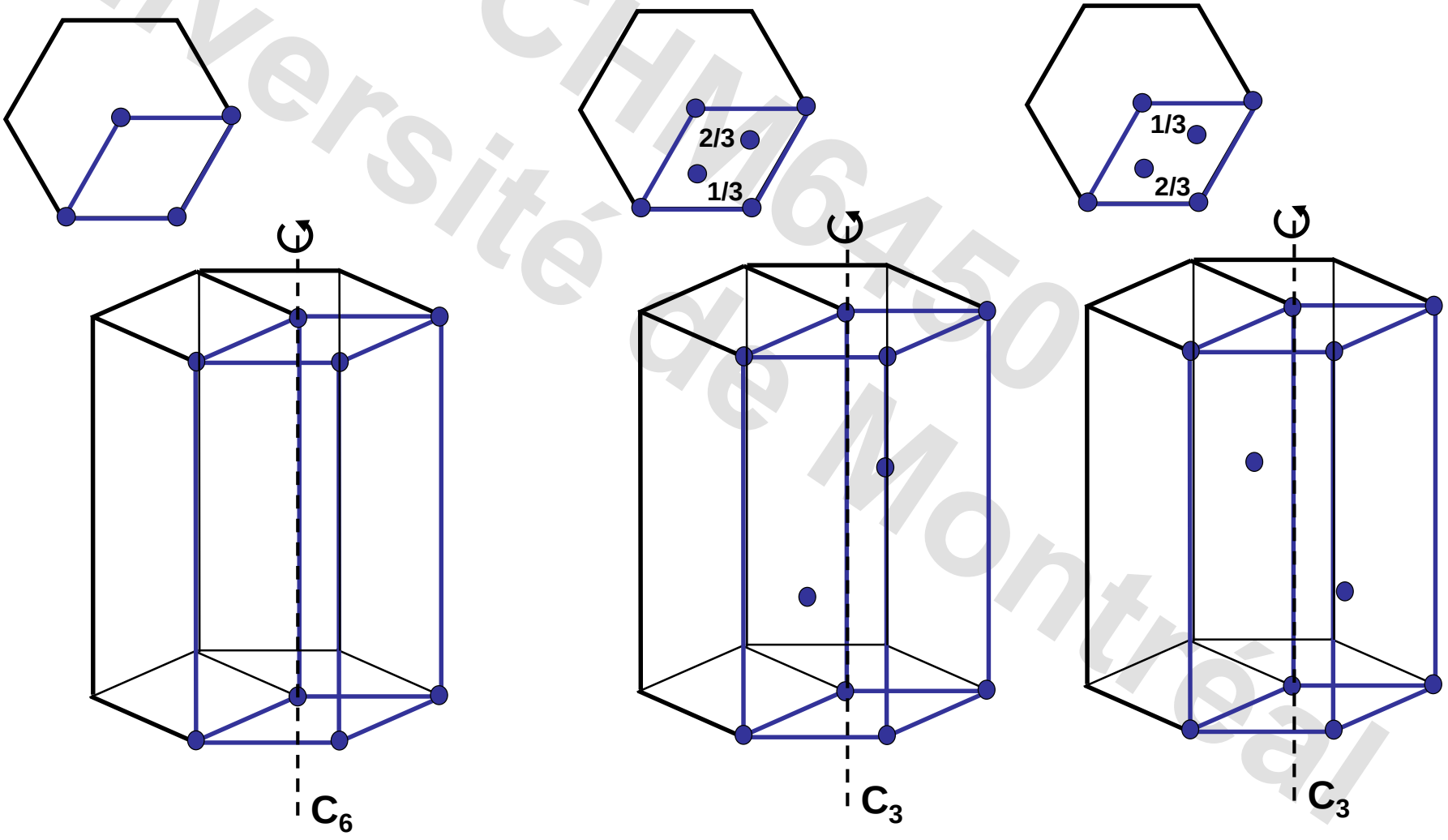






Trigonal, hexagonal, rhomboédrique

We can thus use the hexagonal unit cells for the trigonal crystal systems, which facilitates understanding and calculation.



hP hR (obverse) hR (reverse)

Les 14 réseaux de Bravais («Bravais lattice»)

Triclinic: **aP**

Monoclinic: mP et mC

Orthorhombic: oP, oA, oI, oF

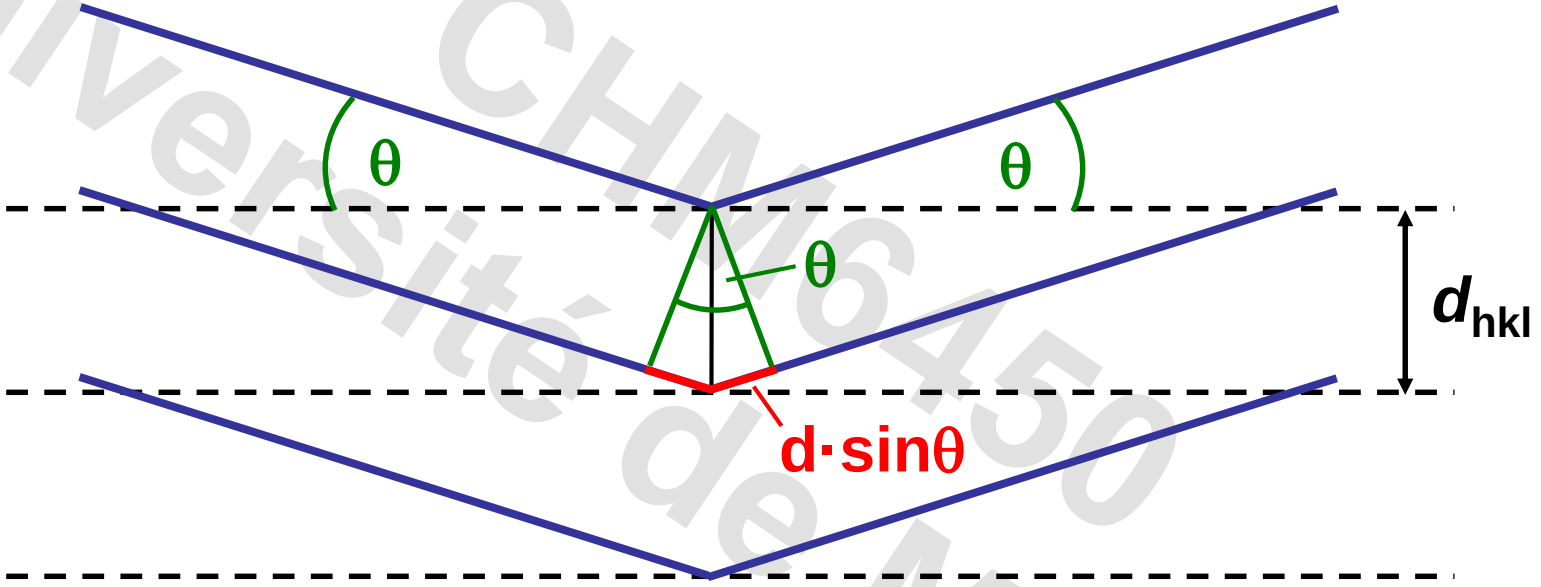
Tetragonal: tP et tI

Trigonal, hexagonal: hP, hR (obverse et reverse)

Cubic: cP, cI et cF

Centered cells have a higher volume than the corresponding primitive cell.

What happens if we increase the size of our unit cell?



Equiangular reflection at the lattice plane *hkl* of the crystal, which obeys the Laue conditions.

Bragg law:

$$2d_{hkl} \cdot \sin\theta = \lambda \quad (n = 1, 2, 3 \ldots)$$

What happens if we increase the size of our unit cell?

Bragg Law:

$$2d_{hkl} \cdot \sin\theta = \lambda \Leftrightarrow \sin\theta = \tfrac{1}{2}\,\lambda\, /\, d_{hkl}$$

Tetragonal unit cell:

a=b=5 Å, **c=10 Å**

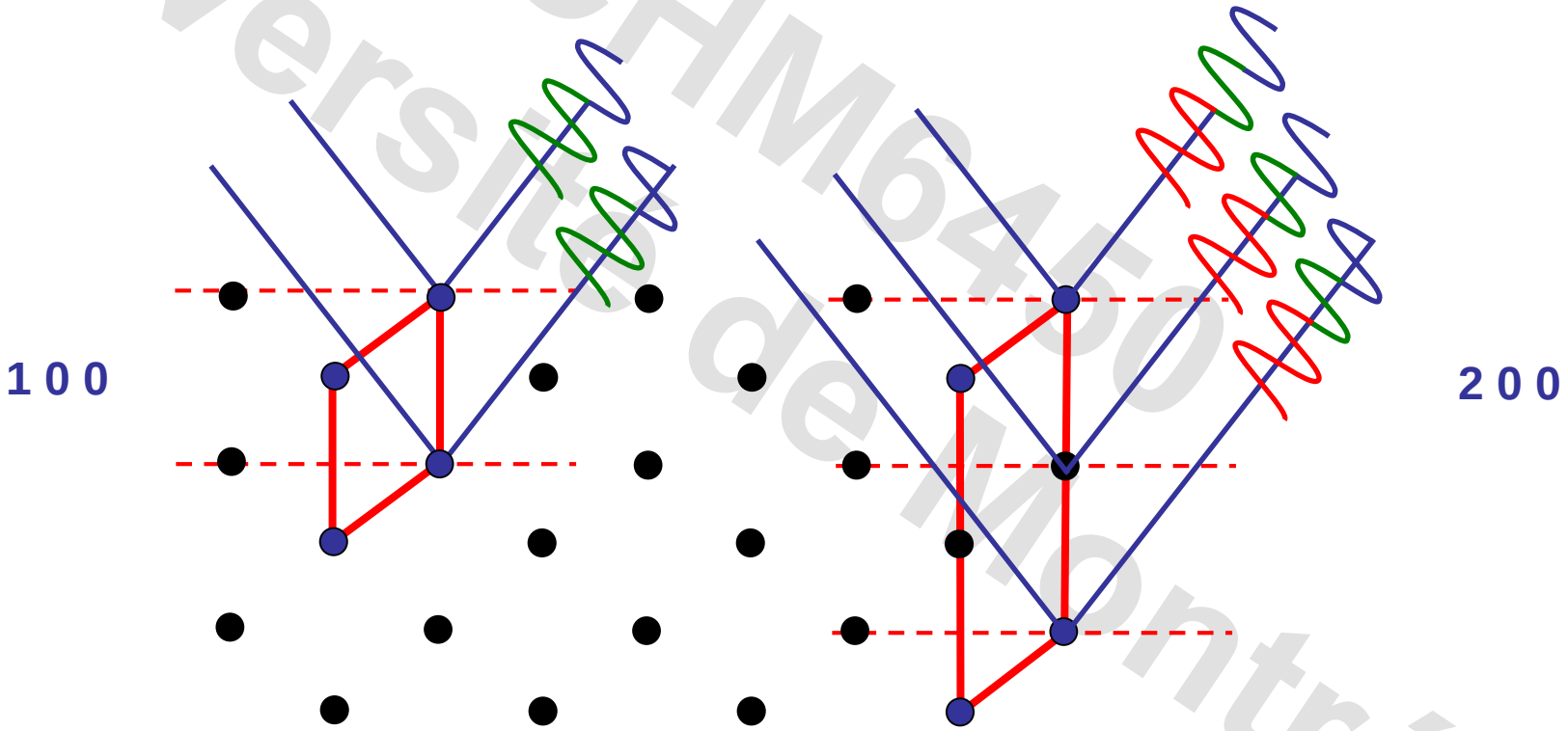
h k l	d_{hkl}	sinθ	θ
0 0 1	10 Å	0.077	4°
0 0 2	5 Å	0.154	9°
0 0 3	3.3 Å	0.231	13°
0 0 4	2.5 Å	0.308	18°
0 0 5	2 Å	0.385	23°

a=b=5 Å, **c=20 Å**

h k l	d_{hkl}	sinθ	θ
0 0 1	20 Å	0.039	2°
0 0 2	10 Å	0.077	4°
0 0 3	6.7 Å	0.116	7°
0 0 4	5 Å	0.154	9°
0 0 5	4 Å	0.193	11°
0 0 6	3.3 Å	0.231	13°
0 0 7	2.9 Å	0.270	16°
0 0 8	2.5 Å	0.308	18°
0 0 9	2.2 Å	0.347	20°
0 0 10	2 Å	0.385	23°
0 0 11	1.8 Å	0.424	25°

What happens if we increase the size of our unit cell?

A unit cell with two times the volume has twice the number of reflections in the same θ region. Can we thus increase the number of reflections by increasing the size of our unit cell?



On doubling the axis length *a* reflection {1 0 0} becomes {2 0 0}.

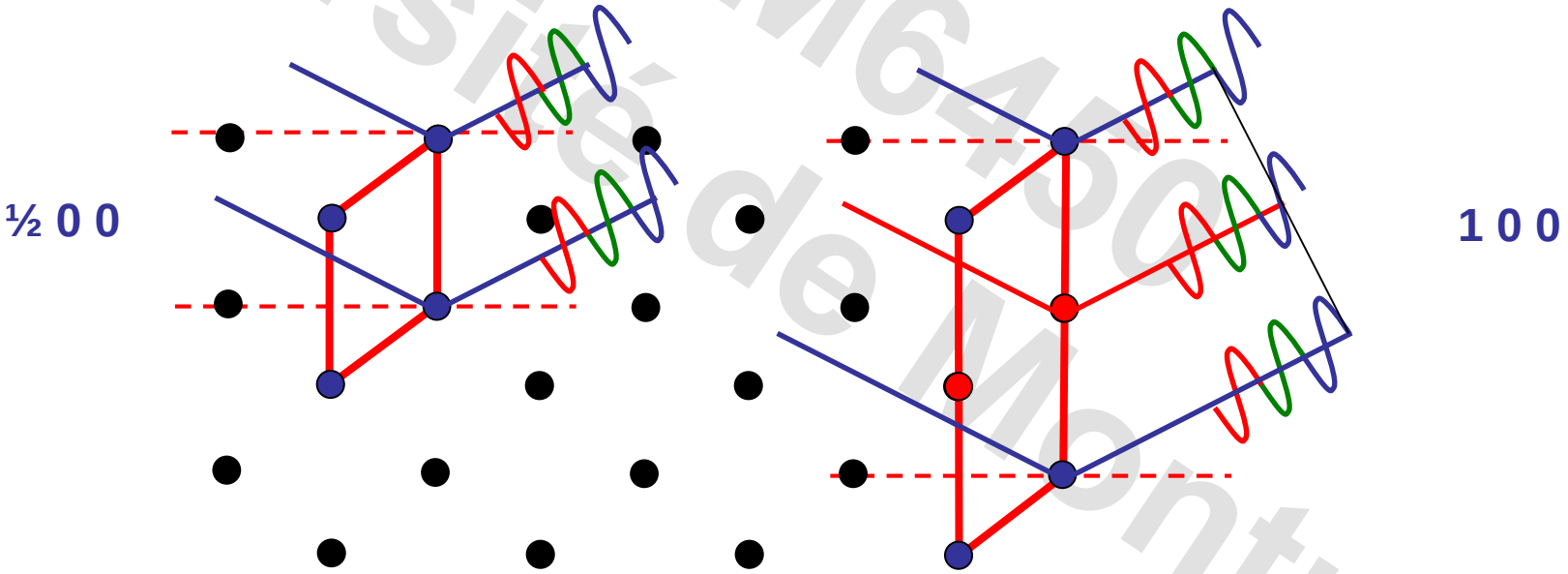
What about the "new" reflection {1 0 0} of our increased unit cell?

What happens if we increase the size of our unit cell?

What about the "new" reflection {1 0 0} of our increased unit cell?

We find systematically another atom at $d_{hkl}/2$. (In other words, we introduced by doubling of the unit cell a new translation operation x+0.5, y, z.).

The path length difference to this atom is ½ λ.



Due to the additional translational symmetry, only reflections with {h k l} with h = 2n are present (path length difference = 2nλ). For reflections {h k l} with odd h, the reflections are systematically absent, since the atom x+0.5 causes destructive interference.

What happens if we increase the size of our unit cell?

Tetragonal unit cell:

a=b=5 Å, **c=10 Å**

h k l	d_{hkl}	sinθ	θ
0 0 1	10 Å	0.077	4°
0 0 2	5 Å	0.154	9°
0 0 3	3.3 Å	0.231	13°
0 0 4	2.5 Å	0.308	18°
0 0 5	2 Å	0.385	23°

a=b=5 Å, **c=20 Å**

h k l	d_{hkl}	sinθ	θ
0 0 1	20 Å	0.039	2°
0 0 2	10 Å	0.077	4°
0 0 3	6.7 Å	0.116	7°
0 0 4	5 Å	0.154	9°
0 0 5	4 Å	0.193	11°
0 0 6	3.3 Å	0.231	13°
0 0 7	2.9 Å	0.270	16°
0 0 8	2.5 Å	0.308	18°
0 0 9	2.2 Å	0.347	20°
0 0 10	2 Å	0.385	23°
0 0 11	1.8 Å	0.424	25°

An artificial increase of an axis length adds new reflections, which are, however, systematically absent (I = 0).

Systematic absences and centering

The introduction of a translational symmetry (**x+0.5**, y, z) causes the systematic absence of all reflections {h k l} with **h ≠ 2n**.

All translational symmetries introduce systematic absences. Since all centering introduce additional translations, centering is associated with the presence of systematic absences, which we can use to **determine** the centering from the reflection list.:

	translation	**Z**	**restrictions**
P	-	1	-
A	x, y+0.5, z+0,5	2	k+l = 2n
B	x+0.5, y, z+0.5	2	h+l = 2n
C	x+0.5, y+0.5, z	2	h+k = 2n
F	**A** + **B** + **C**	4	h+k = 2n, h+l = 2n, k+l = 2n
I	x+0.5, y+0.5, z+0.5	2	h+k+l = 2n

Thus from investigating systematic absences in the reflection list, we can determine the Bravais lattice.

Systematic absences

In the same way, symmetry elements which include translations also cause systematic absences:

Screw axes (axes hélicoïdal):

		translation	restrictions
2_1, 4_2, 6_3	**|| a**	**x+0.5**	**h**00 avec **h = 2n**
	|| b	**y+0.5**	0**k**0 avec **k = 2n**
	|| c	z+0.5	00l avec l = 2n
3_1, 3_2, 6_2, 6_4	|| c	z+**1/3**	00l avec l = **3n**
4_1, 4_3	|| c	z+0.25	00l avec l = 4n
6_1, 6_5	|| c	z+1/6	00l avec l = 6n

Systematic absences

Glide planes:

		translation	zonal restrictions
b	⊥ **a**	**y+0.5**	**0**kl avec **k = 2n**
c	⊥ **a**	**z+0.5**	**0**kl avec **l = 2n**
n	⊥ **a**	**y+0.5, z+0.5**	**0**kl avec **k+l = 2n**
d	⊥ **a**	**y+0.25, z+0.25**	**0**kl avec **k+l = 4n** (F)
c	⊥ **b**	**z+0.5**	h**0**l avec **l = 2n**
a	⊥ **c**	**x+0.5**	hk**0** avec **h = 2n**
c	⊥ **[110]**	**z+0.5**	**hh**l avec **l = 2n** (t, c)
c	⊥ **[120]**	**z+0.5**	**hh**l avec **l = 2n** (trigonal)
d	⊥ **[110]**	**x+0.5, z+0.25**	**hh**l avec **2h+l = 4n** (t, cl)

Space groups

The combination of the translations, defined by the Bravais lattice, and the elements of symmetry possible in an infinite crystal result in the 230 possible space groups. (Group theory: a space group must be closed, i. e. the action of a new element cannot generate an element which is not already in the group.

Example: The most common space group: $P2_1/c$

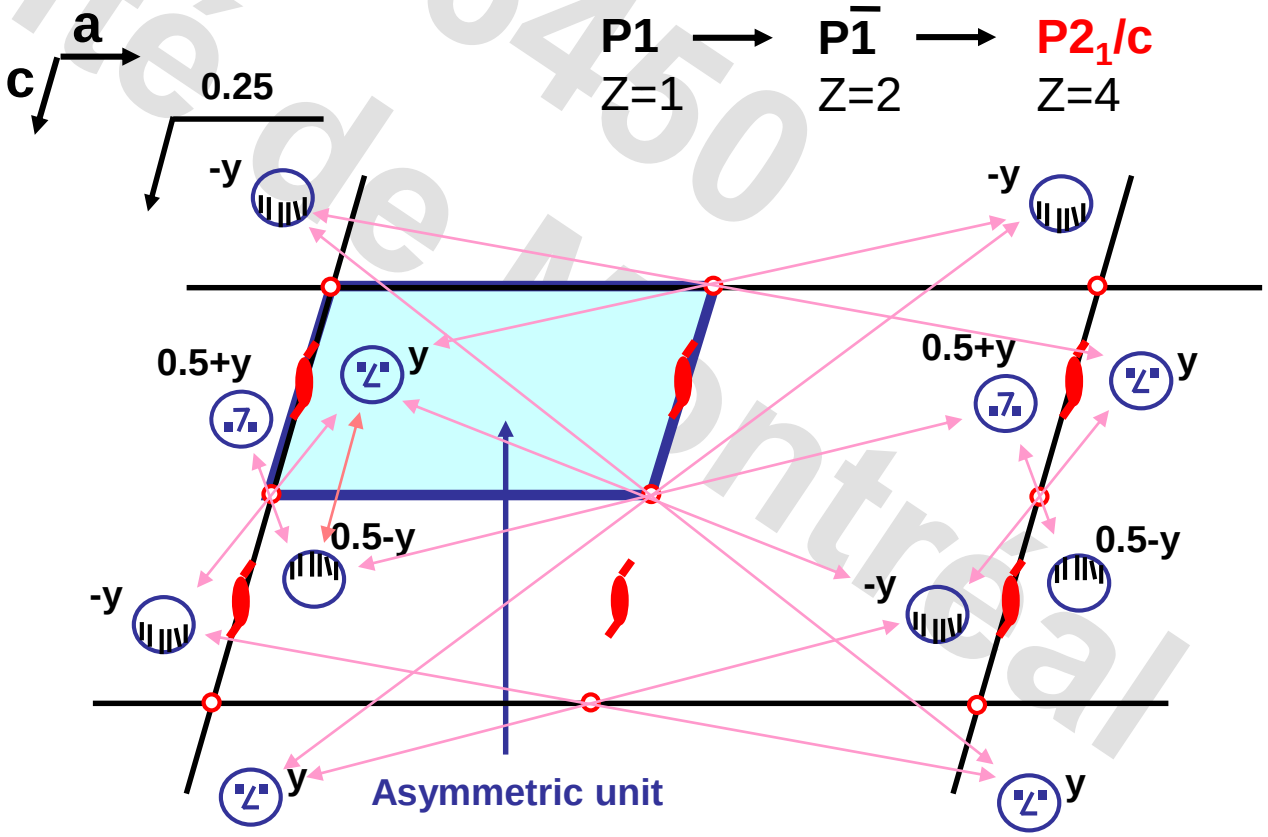
x+1, y, z
x, y+1, z
x, y, z+1

-x, -y, -z *i*

0.5-x, 0.5-y, 0.5-z *i*
0.5-x, y, z *i*
x, 0.5-y, z *i*
x, y, 0.5-z *i*
x, 0.5-y, 0.5-z *i*
0.5-x, y, 0.5-z *i*
0.5-x, 0.5-y, z *i*

x, 0.5-y, z+0.5 *c*

-x, 0.5+y, 0.5-z 2_1



Space group determination

The determination of the correct space group is essential since without a correct description of the symmetry refinement of a structure is not possible (overparametrization or lack of parameters).

To determine the space group we can use the following information:

- **The Laue group (Symmetry of the reflections)**
- **The presence of screw axes and glide planes (systematic absences)**
- **The presence of an inversion center (value E(E-1), chirality of the molecule)**

Crystal systems and Laue group

The combination of the crystal systems with allowed symmetry elements yields 32 crystal classes (or crystallographic point groups):

Crystal system	Crystal class	
Triclinic	C_1	1
	C_i	-1
Monoclinic	C_2	2
	C_s	m
	C_{2h}	2/m
Orthorhombic	D_2	222
	C_{2v}	mm2
	D_{2h}	mmm
Tetragonal	C_4	4
	S_4	-4
	C_{4h}	4/m
	D_4	422
	C_{4v}	4mm
	D_{2d}	-42m
	D_{4h}	4/mmm
Trigonal	C_3	3
	C_{3i}	-3
	D_3	32
	C_{3v}	3m
	D_{3d}	-3m
Hexagonal	C_6	6
	C_{3h}	-6
	C_{6h}	6/m
	D_6	622
	C_{6v}	6mm
	D_{3h}	-6m2
	D_{6h}	6/mmm
Cubic	T	23
	T_h	m3
	O	432
	T_d	-43m
	O_h	m3m

The Laue group results from the combination of crystal class and Friedel's Law

Friedel law

We know that the structure factor is given by:

$$F_{hkl} = \sum_{j=1}^{N} f_j \cdot e^{2\pi i(h\cdot x_j + k\cdot y_j + l\cdot z_j)} = \sum_{j=1}^{N} f_j \cdot e^{i\alpha_j(hkl)}$$

For the inverse reflection (-h -k -l) we obtain: $\alpha_j(\bar{h}\bar{k}\bar{l}) = 2\pi(-h\cdot x_j - k\cdot y_j - l\cdot z_j) = -\alpha_j(hkl)$

$$F_{\bar{h}\bar{k}\bar{l}} = \sum_{j=1}^{N} f_j \cdot e^{i\alpha_j(\bar{h}\bar{k}\bar{l})} = \sum_{j=1}^{N} f_j \cdot e^{-i\alpha_j(hkl)}$$

$$\left|e^{i\varphi}\right|^2 = \cos^2\varphi + \sin^2\varphi; \quad \cos(-\varphi) = \cos(\varphi); \quad \sin(-\varphi) = -\sin(\varphi)$$

$$\left|e^{-i\varphi}\right|^2 = \cos^2(-\varphi) + \sin^2(-\varphi) = \cos^2\varphi + (-\sin\varphi)^2 = \left|e^{i\varphi}\right|^2$$

$$\Rightarrow \quad I_{hkl} = \left|F_{hkl}\right|^2 = I_{\bar{h}\bar{k}\bar{l}}$$

Our reciprocal lattice is thus always centrosymmetric!

32 crystal classes, but 11 Laue groups

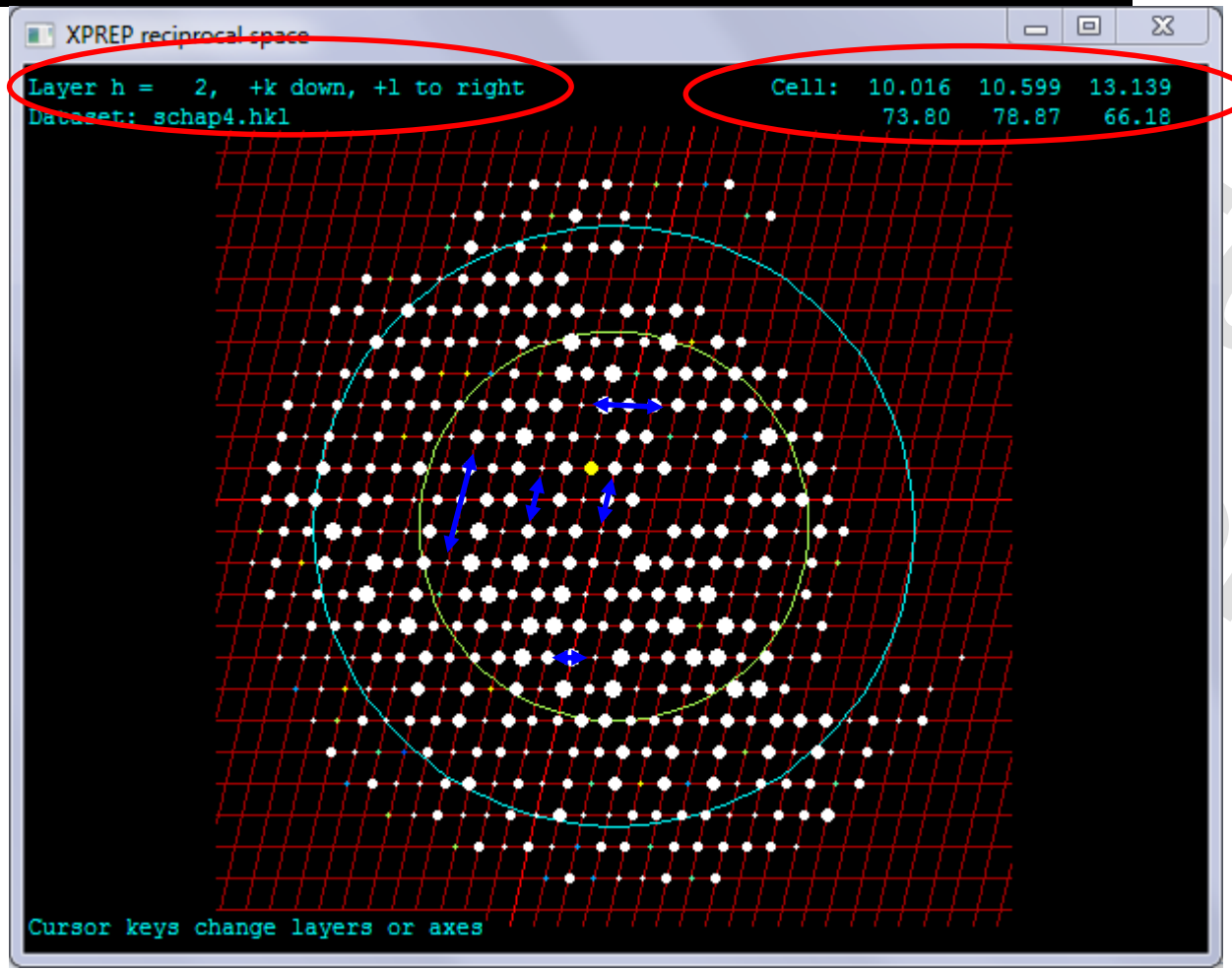
Adding the inversion symmetry caused by Friedel's law, we obtain 11 Laue groups. **The Laue group describes the symmetry of our observed reflections!**

Crystal system	Crystal class		Laue group
Triclinic	C_1	1	**-1**
	C_i	-1	
Monoclinic	C_2	2	**2/m**
	C_s	m	
	C_{2h}	2/m	
Orthorhombic	D_2	222	**mmm**
	C_{2v}	mm2	
	D_{2h}	mmm	
Tetragonal	C_4	4	**4/m**
	S_4	-4	
	C_{4h}	4/m	
	D_4	422	
	C_{4v}	4mm	**4/mmm**
	D_{2d}	-42m	
	D_{4h}	4/mmm	
Trigonal	C_3	3	**-3**
	C_{3i}	-3	
	D_3	32	**-3m1**
	C_{3v}	3m	**-31m**
	D_{3d}	-3m	
Hexagonal	C_6	6	**6/m**
	C_{3h}	-6	
	C_{6h}	6/m	
	D_6	622	**6/mmm**
	C_{6v}	6mm	
	D_{3h}	-6m2	
	D_{6h}	6/mmm	
Cubic	T	23	**m3**
	T_h	m3	
	O	432	**m3m**
	T_d	-43m	
	O_h	m3m	

Visualisation of reciprocal space with XPREP

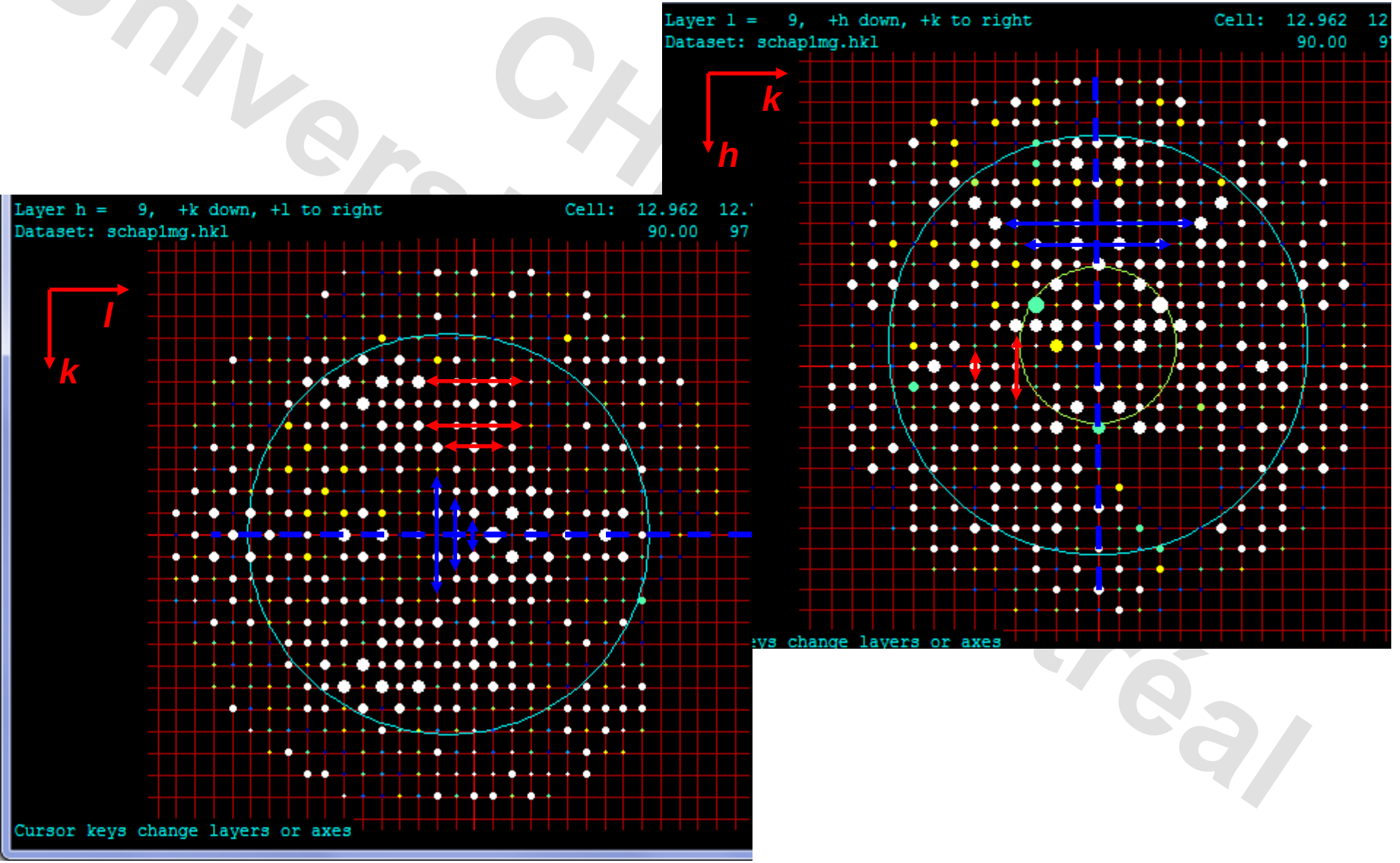
```
[D] Read, modify or merge DATASETS          [C] Define unit-cell CONTENTS
[P] Contour PATTERSON sections              [F] Set up shelxtl FILES
[H] Search for HIGHER metric symmetry       [R] RECIPROCAL space displays
[S] Determine or input SPACE GROUP          [U] UNIT-CELL transformations
[A] Absorption, powder, SIR, SAD, MAD etc.  [T] Change TOLERANCES
[M] Test for MEROHEDRAL TWINNING            [O] Self-rotation function
[L] Reset LATTICE type of original cell     [Q] QUIT program

Select option [D]:
```



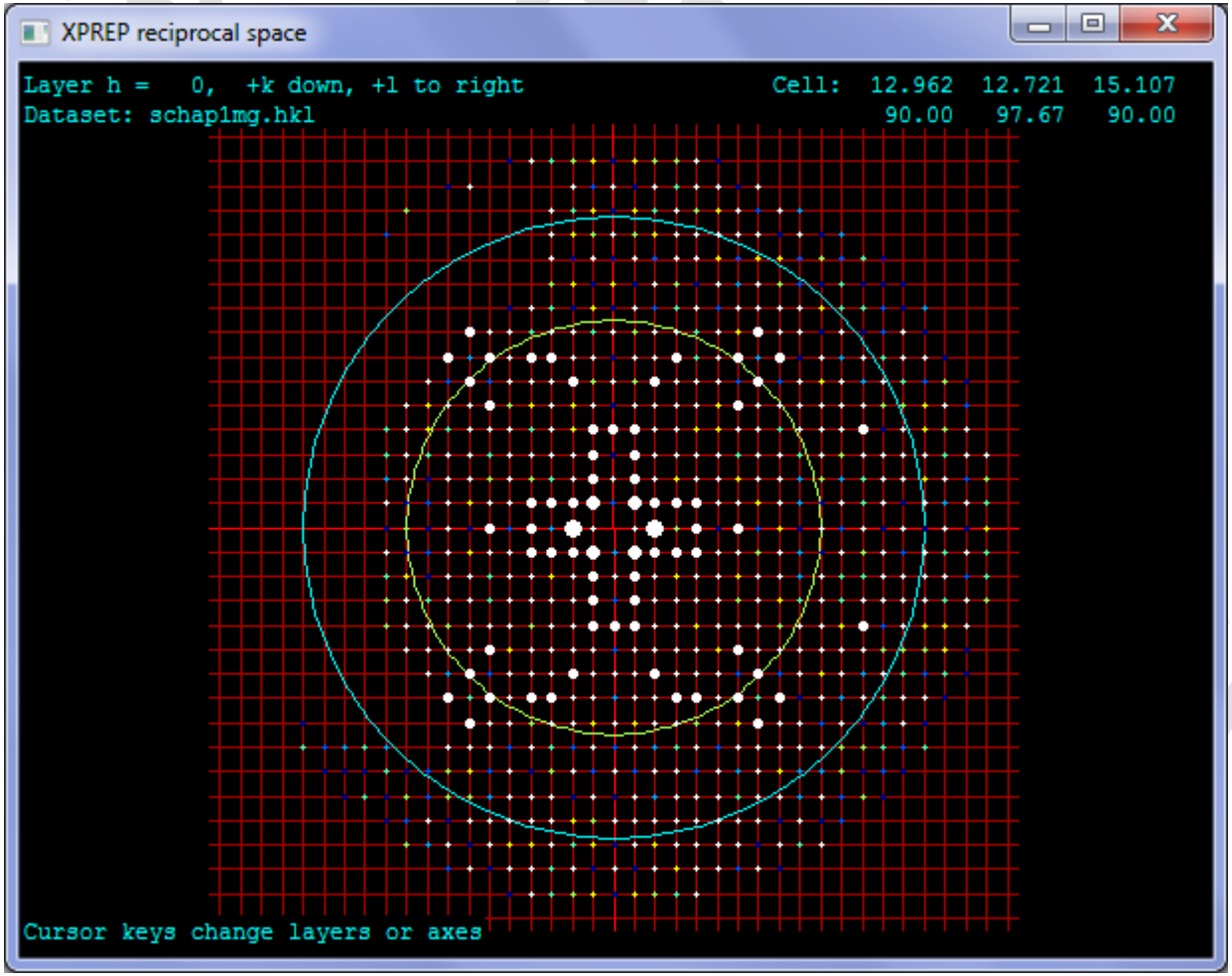
Triclinic:
No symétrie but inversion (Friedel's Law)

Monoclinic: hkl = h –k l, mirror plane perpendicular to k

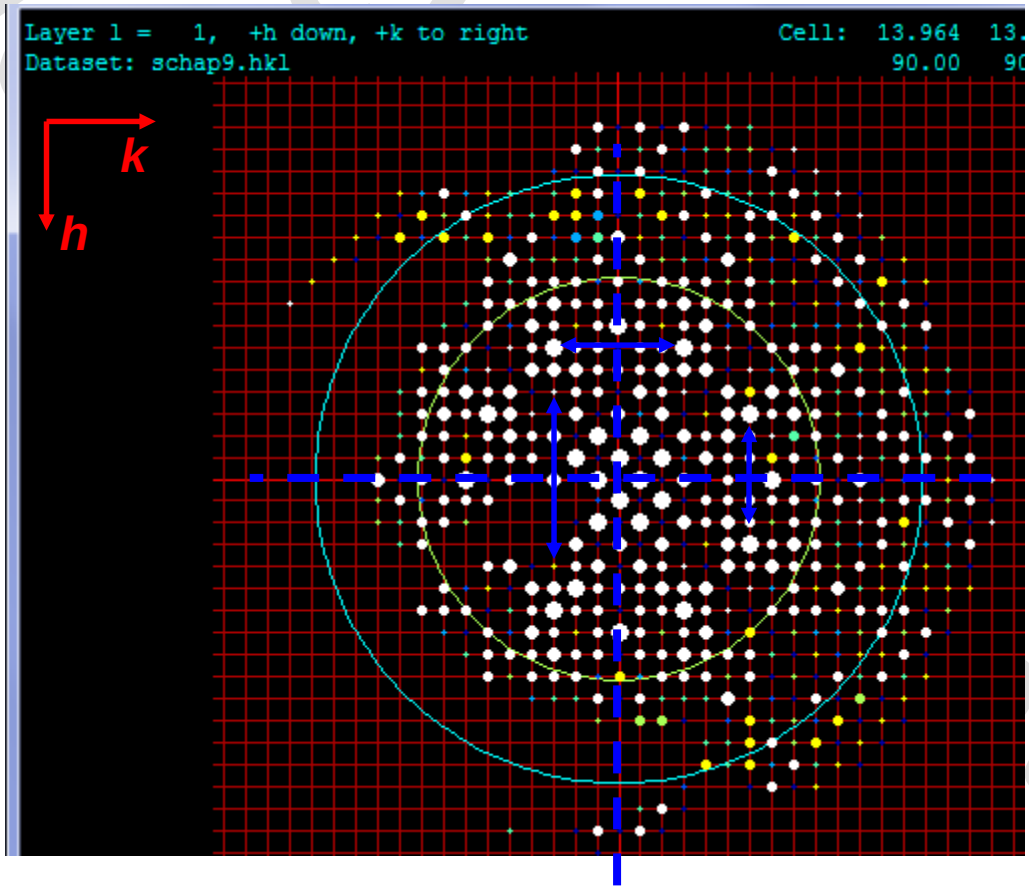


Monoclinic: hkl = h –k l, mirror plane perpendicular to k

Avoid planes with h=0, k=0 or l=0, since h = -h is trivial for h = 0



Tetragonal: Two Laue groups: 4/m or 4/mmm:
4-fold axis parallel to *l*, either mirror plane perpendicular to *l* or at all axes



Here: 4/mmm

Space group determination

The determination of the correct space group is essential since – without a correct description of the symmetry – neither the solution nor the refinement of a structure is possible..

To determine the space group we can use the following information:

- **The Laue group (Symmetry of the reflections)**
- **The presence of screw axes and glide planes (systematic absences)**
- **The presence of an inversion center (value E(E-1), chirality of the molecule)**

Systematic absences

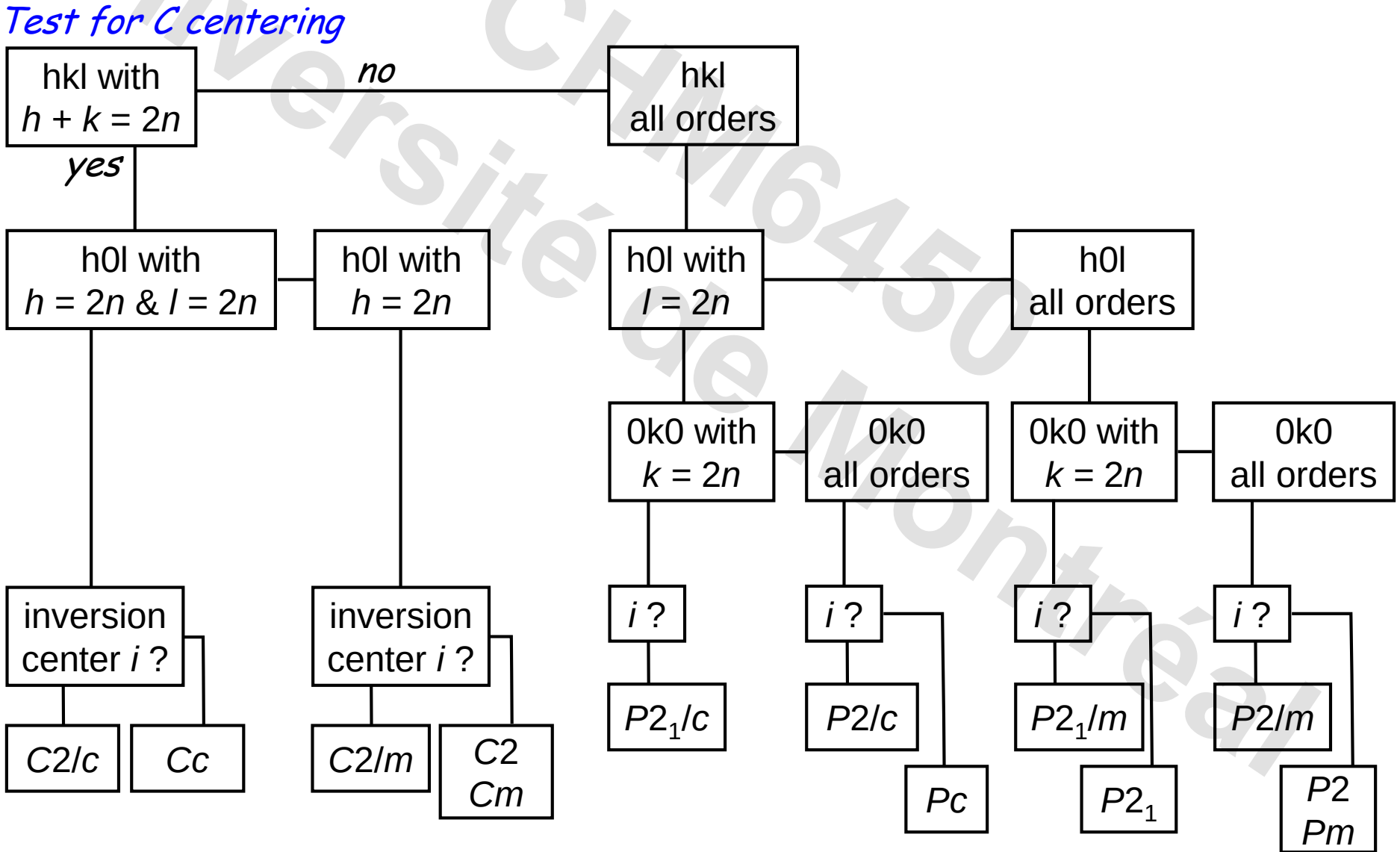
- **Determination which screw axes and glide planes are present.**
- **Determination which space groups contain these symmetry elements.**

- **By hand**
  - Use the provided tables (Studium)
  - Start always at the end of a table (most special case) and work towards the more general ones
  - Check if the reflection condition mentioned is violated. I. e. h00: h = 2n: check if there are several reflections h00 with odd h, which have a intensities higher than 3σ. About 10% of errors are allowed. Thus if in 20 systematic absences, you find two which are >3σ, the reflection condition might be nevertheless valid.
  - Once you find which table A, B, C… you are in, go to the subtable. Start again at the end.

Space group determination by hand

Example Vivan8:

a = 30.8391(7) Å, *b* = 14.2009(4) Å, *c* = 29.0930(7) Å, **α = 90°**, β = 119.0730(10)°, **γ = 90°**



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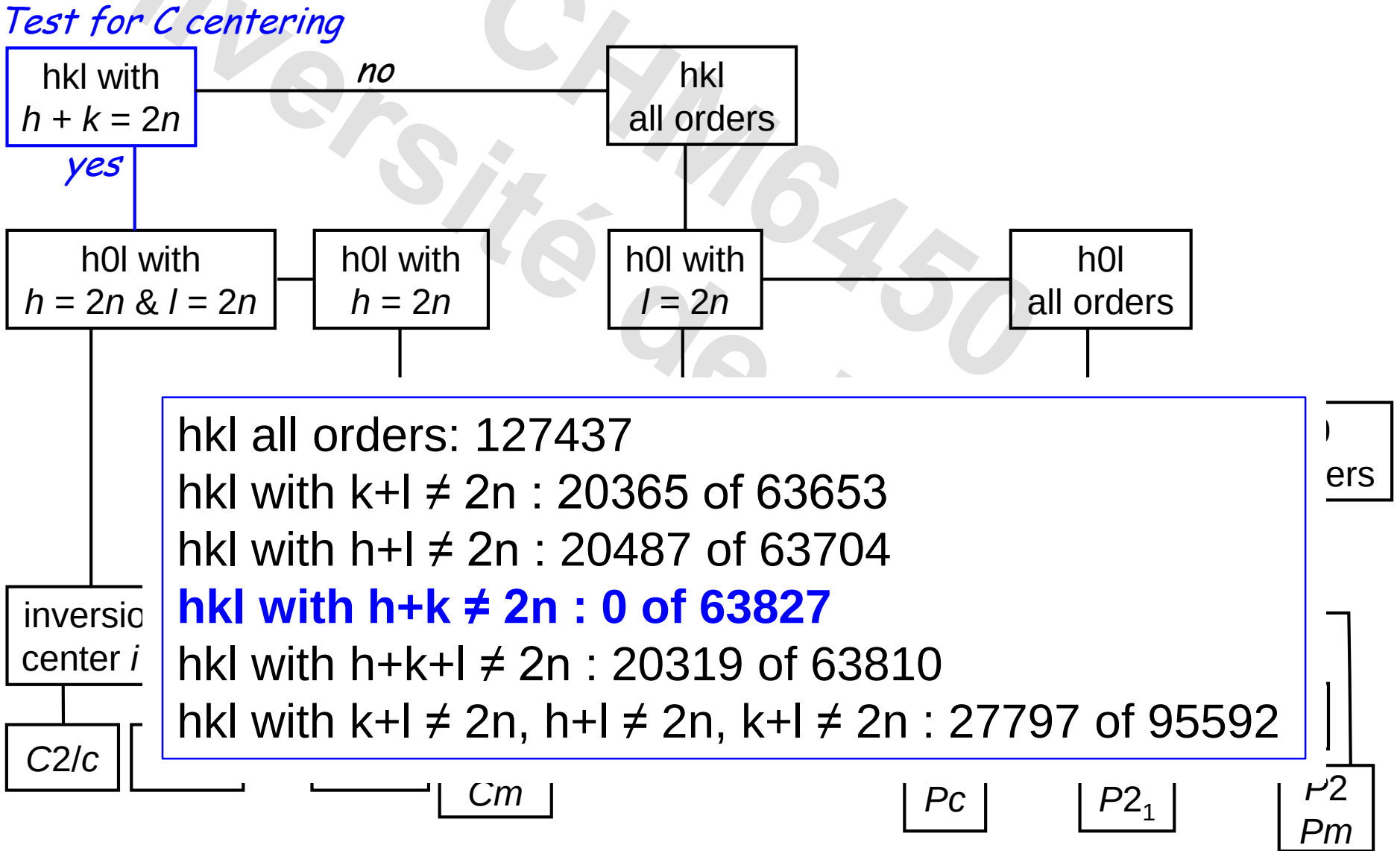

Space group determination by hand

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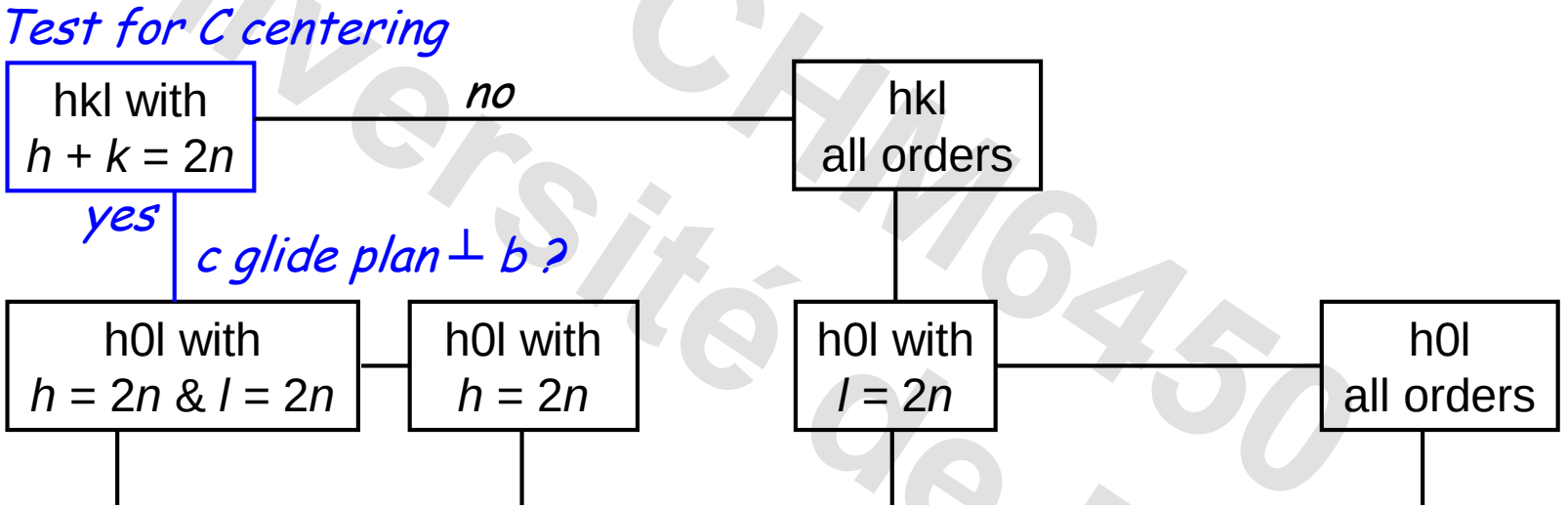
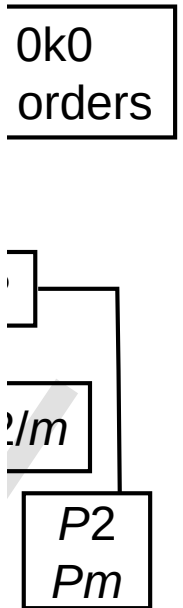


h	k	l	I	sigma	h	k	l	I	sigma	h	k	l	I	sigma	h	k	l	I	sigma	h	k	l	I	sigma
0	**0**	**-1**	**0**	**0.01**	**0**	**0**	**-17**	**-0.04**	**0.1**	**1**	**0**	**5**	**0.04**	**0.04**	**2**	**0**	**9**	**-0.04**	**0.04**					
0	0	-2	0.4	0.02	0	0	-18	0.37	0.11	**1**	**0**	**4**	**-0.02**	**0.03**	2	0	8	1.34	0.07					
0	**0**	**-3**	**-0.01**	**0.02**	**1**	**0**	**19**	**-0.09**	**0.1**	**1**	**0**	**3**	**0.06**	**0.02**	**2**	**0**	**7**	**-0.03**	**0.04**					
0	0	-4	127	0.47	**1**	**0**	**18**	**-0.17**	**0.09**	**1**	**0**	**2**	**0**	**0.02**	2	0	6	100.11	0.41					
0	**0**	**-5**	**-0.02**	**0.03**	**1**	**0**	**17**	**0.02**	**0.11**	**1**	**0**	**1**	**0.02**	**0.01**	**2**	**0**	**5**	**-0.04**	**0.04**	**3**	**0**	**12**	**-0.05**	**0.08**
0	0	-6	10.16	0.11	**1**	**0**	**16**	**-0.13**	**0.09**	**1**	**0**	**0**	**0**	**0.01**	2	0	4	209.88	0.78	**3**	**0**	**11**	**1.52**	**0.11**
0	**0**	**-7**	**-0.03**	**0.04**	**1**	**0**	**15**	**0.69**	**0.13**	**2**	**0**	**19**	**-0.11**	**0.11**	**2**	**0**	**3**	**-0.01**	**0.03**	**3**	**0**	**10**	**0**	**0.05**
0	0	-8	269.59	0.97	**1**	**0**	**14**	**-0.01**	**0.09**	2	0	18	13.37	0.28	2	0	2	17.97	0.11	**3**	**0**	**9**	**-0.03**	**0.05**
0	**0**	**-9**	**-0.03**	**0.04**	**1**	**0**	**13**	**0.18**	**0.1**	**2**	**0**	**17**	**-0.07**	**0.09**	**2**	**0**	**1**	**-0.01**	**0.02**	**3**	**0**	**8**	**-0.01**	**0.04**
0	0	-10	0.75	0.07	**1**	**0**	**12**	**0**	**0.06**	2	0	16	19.37	0.39	2	0	0	251.03	1.01	**3**	**0**	**7**	**0.02**	**0.04**
0	**0**	**-11**	**0.02**	**0.05**	**1**	**0**	**11**	**1.49**	**0.09**	**2**	**0**	**15**	**-0.11**	**0.09**	**3**	**0**	**18**	**-0.06**	**0.11**	**3**	**0**	**6**	**-0.01**	**0.04**
0	0	-12	449.53	1.41	**1**	**0**	**10**	**-0.06**	**0.04**	2	0	14	20.21	0.36	**3**	**0**	**17**	**-0.02**	**0.1**	**3**	**0**	**5**	**0.16**	**0.04**
0	**0**	**-13**	**-0.07**	**0.06**	**1**	**0**	**9**	**0**	**0.04**	**2**	**0**	**13**	**-0.12**	**0.08**	**3**	**0**	**16**	**-0.09**	**0.11**	**3**	**0**	**4**	**-0.02**	**0.04**
0	0	-14	25.88	0.38	**1**	**0**	**8**	**-0.02**	**0.04**	2	0	12	127.11	0.69	**3**	**0**	**15**	**-0.04**	**0.1**	**3**	**0**	**3**	**0.45**	**0.04**
0	**0**	**-15**	**-0.12**	**0.08**	**1**	**0**	**7**	**0.84**	**0.06**	**2**	**0**	**11**	**-0.09**	**0.05**	**3**	**0**	**14**	**-0.02**	**0.1**	**3**	**0**	**2**	**0**	**0.03**
0	0	-16	135.75	0.98	**1**	**0**	**6**	**-0.03**	**0.04**	2	0	10	26.69	0.23	**3**	**0**	**13**	**0.05**	**0.09**	**3**	**0**	**1**	**0.13**	**0.03**



Space group determination by hand

Example Vivan8:

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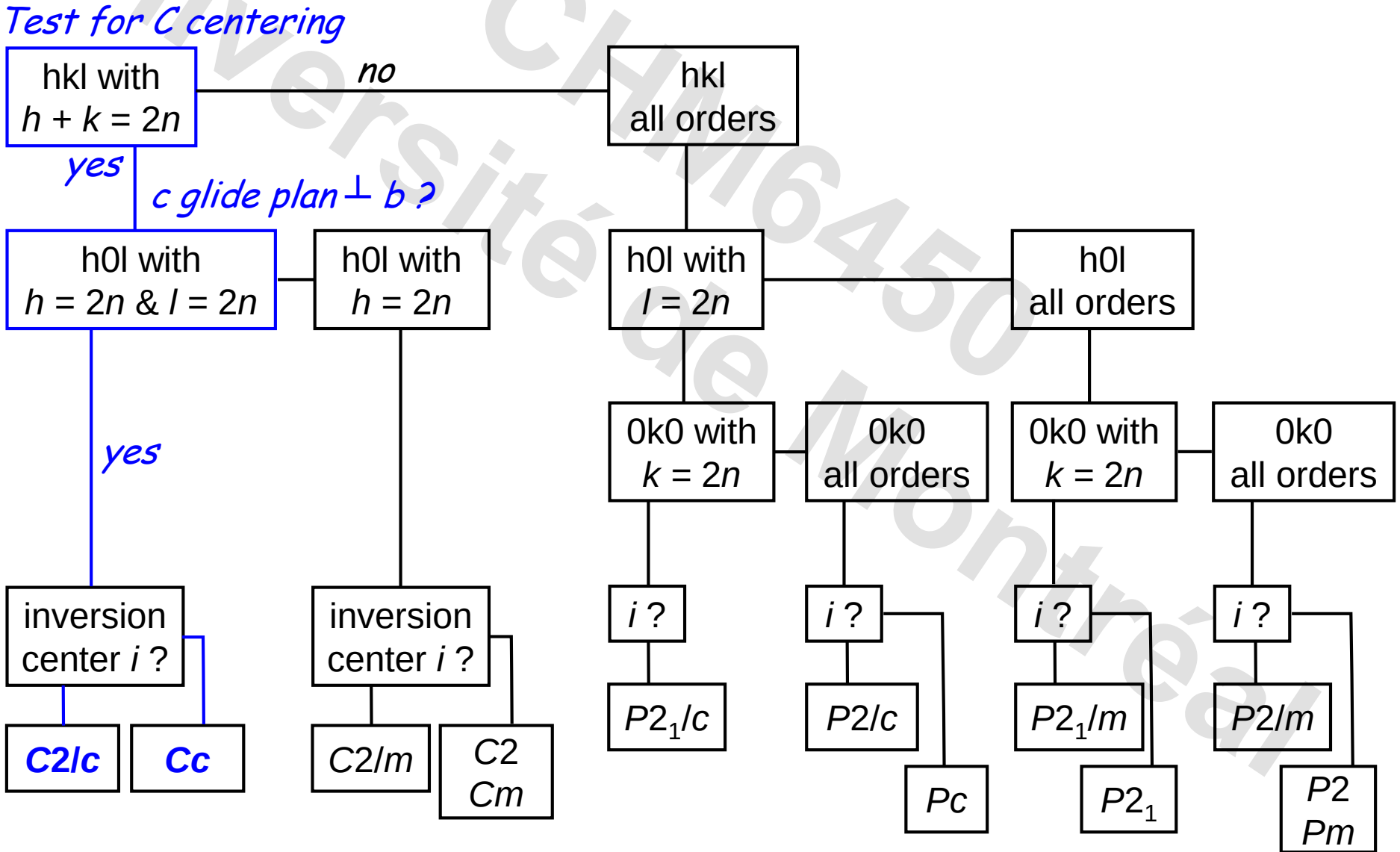

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, *b* = 17.4848(3) Å, *c* = 8.9597(2) Å, **α = 90°**, **β = 90°**, **γ = 90°**

Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n*	hkl with *h*+*k*+l = 2*n*	hkl with *h* + l = 2*n*	hkl with *k* + l = 2*n*	hkl with *h* + l = 2*n*	hkl all orders
F	***I***	***B***	***A***	***C***	***P***

Lattice exceptions	P	A *k*+*l*=2*n*	B *h*+*l*=2*n*	C *h*+*k*=2*n*	I *h*+*k*+*l*=2*n*	F *k*+*l*, *h*+*l*, *h*+*k*=2*n*	All
Total no. Reflections	0	18455	18302	18397	18426	27577	36770
Total with I>3sig(I)	0	14415	14946	14937	14677	22149	30028
Mean I/sig(I) (all)	0.0	10.1	10.5	10.5	10.3	10.3	**10.5**
Mean I/sig(I) I>3sig(I)	0.0	12.6	12.6	12.7	12.7	12.6	**12.6**

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, *b* = 17.4848(3) Å, *c* = 8.9597(2) Å, **α = 90°**, **β = 90°**, **γ = 90°**

Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n*	hkl with *h*+*k*+l = 2*n*	hkl with *h* + *l* = 2*n*	hkl with *k* + *l* = 2*n*	hkl with *h* + *k* = 2*n*	hkl all orders
F	***I***	***B***	***A***	***C***	***P***

glide plan ⊥ a ?

0kl with *l* = 2*n*	0kl with *k* = 2*n*	0kl with *k* + *l* = 2*n*	0kl all orders
Pc			

0	0	1	0,01	0,01	0	2	1	0,02	0,01	0	3	10	-0,04	0,05	0	5	5	**20,89**	0,33
0	0	2	**57,86**	1,17	0	2	2	**12,96**	0,17	0	4	0	**6,19**	0,13	0	5	6	0	0,05
0	0	3	-0,01	0,02	0	2	3	0,02	0,01	0	4	1	0,01	0,02	0	5	7	**20,26**	0,42
0	0	4	**48,76**	0,99	0	2	4	**96,14**	1,37	0	4	2	**917,7**	12,9	0	5	8	-0,01	0,07
0	0	5	0	0,03	0	2	5	0	0,02	0	4	3	0	0,01	0	5	9	**2,57**	0,13
0	0	6	**26,39**	0,74	0	2	6	**57,37**	1,18	0	4	4	**38,66**	0,49	0	5	10	-0,05	0,05
0	0	7	-0,06	0,07	0	2	7	-0,05	0,05	0	4	5	0,04	0,03	0	6	0	**4,11**	0,11
0	0	8	**12,9**	0,8	0	2	8	**16,17**	0,42	0	4	6	**9,81**	0,26	0	6	1	0,03	0,02
0	0	9	-0,13	0,1	0	2	9	-0,07	0,07	0	4	7	-0,02	0,05	0	6	2	**91,44**	1,3
0	0	10	**1,64**	0,15	0	2	10	**5,59**	0,21	0	4	8	**3,84**	0,14	0	6	3	0,02	0,02
0	1	0	0,02	0,01	0	3	0	0,01	0,01	0	4	9	0	0,07	0	6	4	**7,84**	0,13
0	1	1	**261,7**	3,41	0	3	1	**24,79**	0,38	0	4	10	**3,53**	0,14	0	6	5	0,03	0,03
0	1	2	0,01	0,01	0	3	2	0	0,01	0	5	0	0	0,02	0	6	6	**29,02**	0,46
0	1	3	**14,24**	0,2	0	3	3	**167,8**	1,93	0	5	1	**292**	4,1	0	6	7	0,08	0,07
0	1	4	0,03	0,02	0	3	4	0	0,02	0	5	2	0	0,02	0	6	8	**3,42**	0,15
0	1	5	**38,4**	0,59	0	3	5	**25,77**	0,47	0	5	3	**9,78**	0,14	0	6	9	0,02	0,07
0	1	6	0	0,04	0	3	6	0,04	0,04	0	5	4	0,04	0,02	0	6	10	**8,95**	0,26
0	1	7	**10,88**	0,21	0	3	7	**15,01**	0,26										
0	1	8	0,01	0,07	0	3	8	0,01	0,08										
0	1	9	**7,38**	0,23	0	3	9	**4,4**	0,2										
0	1	10	-0,01	0,06															
0	2	0	**166,8**	3,02															

0	6	10	**8,95**	0,26	0	8	5	-0,02	0,04
0	7	0	0,03	0,03	0	8	6	**2,07**	0,08
0	7	1	**36,27**	0,55	0	8	7	-0,02	0,07
0	7	2	-0,01	0,02	0	8	8	**3,2**	0,13
0	7	3	**19,62**	0,32	0	8	9	0,04	0,06
0	7	4	0	0,02	0	9	0	0,04	0,04
0	7	5	**30,68**	0,47	0	9	1	**8,7**	0,17
0	7	6	0,01	0,04	0	9	2	0	0,03
0	7	7	**15,08**	0,37	0	9	3	**33,21**	0,56
0	7	8	0,02	0,07	0	9	4	-0,01	0,03
0	7	9	**2,87**	0,12	0	9	5	**13,61**	0,2
0	7	10	0,01	0,05	0	9	6	-0,04	0,08
0	8	0	**3,62**	0,12	0	9	7	**10,61**	0,27
0	8	1	0,02	0,02	0	9	8	0,01	0,06
0	8	2	**6,89**	0,13	0	9	9	**1,89**	0,09
0	8	3	-0,02	0,03					
0	8	4	**311,2**	4,2					

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, *b* = 17.4848(3) Å, *c* = 8.9597(2) Å, **α = 90°**, **β = 90°**, **γ = 90°**

Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n*	hkl with *h*+*k*+l = 2*n*	hkl with *h* + *l* = 2*n*	hkl with *k* + *l* = 2*n*	hkl with *h* + *k* = 2*n*	hkl all orders
F	***I***	***B***	***A***	***C***	***P***

glide plan ⊥ a ?

0kl with *l* = 2*n*	0kl with *k* = 2*n*	0kl with *k* + *l* = 2*n*	0kl all orders
Pc__	*Pb__*		

0	0	1	0,01	0,01
0	0	2	**57,86**	1,17
0	0	3	-0,01	0,02
0	0	4	**48,76**	0,99
0	0	5	0	0,03
0	0	6	**26,39**	0,74
0	0	7	-0,06	0,07
0	0	8	**12,9**	0,8
0	0	9	-0,13	0,1
0	0	10	**1,64**	0,15
0	1	0	0,02	0,01
0	1	1	**261,7**	3,41
0	1	2	0,01	0,01
0	1	3	**14,24**	0,2
0	1	4	0,03	0,02
0	1	5	**38,4**	0,59
0	1	6	0	0,04
0	1	7	**10,88**	0,21
0	1	8	0,01	0,07
0	1	9	**7,38**	0,23
0	1	10	-0,01	0,06
0	2	0	**166,8**	3,02

0	2	1	0,02	0,01
0	2	2	**12,96**	0,17
0	2	3	0,02	0,01
0	2	4	**96,14**	1,37
0	2	5	0	0,02
0	2	6	**57,37**	1,18
0	2	7	-0,05	0,05
0	2	8	**16,17**	0,42
0	2	9	-0,07	0,07
0	2	10	**5,59**	0,21
0	3	0	0,01	0,01
0	3	1	**24,79**	0,38
0	3	2	0	0,01
0	3	3	**167,8**	1,93
0	3	4	0	0,02
0	3	5	**25,77**	0,47
0	3	6	0,04	0,04
0	3	7	**15,01**	0,26
0	3	8	0,01	0,08
0	3	9	**4,4**	0,2

0	3	10	-0,04	0,05
0	4	0	**6,19**	0,13
0	4	1	0,01	0,02
0	4	2	**917,7**	12,9
0	4	3	0	0,01
0	4	4	**38,66**	0,49
0	4	5	0,04	0,03
0	4	6	**9,81**	0,26
0	4	7	-0,02	0,05
0	4	8	**3,84**	0,14
0	4	9	0	0,07
0	4	10	**3,53**	0,14
0	5	0	0	0,02
0	5	1	**292**	4,1
0	5	2	0	0,02
0	5	3	**9,78**	0,14
0	5	4	0,04	0,02

0	5	5	**20,89**	0,33
0	5	6	0	0,05
0	5	7	**20,26**	0,42
0	5	8	-0,01	0,07
0	5	9	**2,57**	0,13
0	5	10	-0,05	0,05
0	6	0	**4,11**	0,11
0	6	1	0,03	0,02
0	6	2	**91,44**	1,3
0	6	3	0,02	0,02
0	6	4	**7,84**	0,13
0	6	5	0,03	0,03
0	6	6	**29,02**	0,46
0	6	7	0,08	0,07
0	6	8	**3,42**	0,15
0	6	9	0,02	0,07
0	6	10	**8,95**	0,26

0	6	10	**8,95**	0,26
0	7	0	0,03	0,03
0	7	1	**36,27**	0,55
0	7	2	-0,01	0,02
0	7	3	**19,62**	0,32
0	7	4	0	0,02
0	7	5	**30,68**	0,47
0	7	6	0,01	0,04
0	7	7	**15,08**	0,37
0	7	8	0,02	0,07
0	7	9	**2,87**	0,12
0	7	10	0,01	0,05
0	8	0	**3,62**	0,12
0	8	1	0,02	0,02
0	8	2	**6,89**	0,13
0	8	3	-0,02	0,03
0	8	4	**311,2**	4,2

0	8	5	-0,02	0,04
0	8	6	**2,07**	0,08
0	8	7	-0,02	0,07
0	8	8	**3,2**	0,13
0	8	9	0,04	0,06
0	9	0	0,04	0,04
0	9	1	**8,7**	0,17
0	9	2	0	0,03
0	9	3	**33,21**	0,56
0	9	4	-0,01	0,03
0	9	5	**13,61**	0,2
0	9	6	-0,04	0,08
0	9	7	**10,61**	0,27
0	9	8	0,01	0,06
0	9	9	**1,89**	0,09

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F	***I***	***B***	***A***	***C***	***P***

glide plan ⊥ a ?

0kl with *l* = 2*n*	0kl with *k* = 2*n*	0kl with *k* + *l* = 2*n*	0kl all orders
Pc__	*Pb__*	*Pn__*	

0	0	1	0,01	0,01	0	2	1	0,02	0,01	0	3	10	-0,04	0,05	0	5	5	**20,89**	0,33	0	6	10	**8,95**	0,26	0	8	5	-0,02	0,04
0	0	2	**57,86**	1,17	0	2	2	**12,96**	0,17	0	4	0	**6,19**	0,13	0	5	6	0	0,05	0	7	0	0,03	0,03	0	8	6	**2,07**	0,08
0	0	3	-0,01	0,02	0	2	3	0,02	0,01	0	4	1	0,01	0,02	0	5	7	**20,26**	0,42	0	7	1	**36,27**	0,55	0	8	7	-0,02	0,07
0	0	4	**48,76**	0,99	0	2	4	**96,14**	1,37	0	4	2	**917,7**	12,9	0	5	8	-0,01	0,07	0	7	2	-0,01	0,02	0	8	8	**3,2**	0,13
0	0	5	0	0,03	0	2	5	0	0,02	0	4	3	0	0,01	0	5	9	**2,57**	0,13	0	7	3	**19,62**	0,32	0	8	9	0,04	0,06
0	0	6	**26,39**	0,74	0	2	6	**57,37**	1,18	0	4	4	**38,66**	0,49	0	5	10	-0,05	0,05	0	7	4	0	0,02	0	9	0	0,04	0,04
0	0	7	-0,06	0,07	0	2	7	-0,05	0,05	0	4	5	0,04	0,03	0	6	0	**4,11**	0,11	0	7	5	**30,68**	0,47	0	9	1	**8,7**	0,17
0	0	8	**12,9**	0,8	0	2	8	**16,17**	0,42	0	4	6	**9,81**	0,26	0	6	1	0,03	0,02	0	7	6	0,01	0,04	0	9	2	0	0,03
0	0	9	-0,13	0,1	0	2	9	-0,07	0,07	0	4	7	-0,02	0,05	0	6	2	**91,44**	1,3	0	7	7	**15,08**	0,37	0	9	3	**33,21**	0,56
0	0	10	**1,64**	0,15	0	2	10	**5,59**	0,21	0	4	8	**3,84**	0,14	0	6	3	0,02	0,02	0	7	8	0,02	0,07	0	9	4	-0,01	0,03
0	1	0	0,02	0,01	0	3	0	0,01	0,01	0	4	9	0	0,07	0	6	4	**7,84**	0,13	0	7	9	**2,87**	0,12	0	9	5	**13,61**	0,2
0	1	1	**261,7**	3,41	0	3	1	**24,79**	0,38	0	4	10	**3,53**	0,14	0	6	5	0,03	0,03	0	7	10	0,01	0,05	0	9	6	-0,04	0,08
0	1	2	0,01	0,01	0	3	2	0	0,01	0	5	0	0	0,02	0	6	6	**29,02**	0,46	0	8	0	**3,62**	0,12	0	9	7	**10,61**	0,27
0	1	3	**14,24**	0,2	0	3	3	**167,8**	1,93	0	5	1	**292**	4,1	0	6	7	0,08	0,07	0	8	1	0,02	0,02	0	9	8	0,01	0,06
0	1	4	0,03	0,02	0	3	4	0	0,02	0	5	2	0	0,02	0	6	8	**3,42**	0,15	0	8	2	**6,89**	0,13	0	9	9	**1,89**	0,09
0	1	5	**38,4**	0,59	0	3	5	**25,77**	0,47	0	5	3	**9,78**	0,14	0	6	9	0,02	0,07	0	8	3	-0,02	0,03					
0	1	6	0	0,04	0	3	6	0,04	0,04	0	5	4	0,04	0,02	0	6	10	**8,95**	0,26	0	8	4	**311,2**	4,2					
0	1	7	**10,88**	0,21	0	3	7	**15,01**	0,26																				
0	1	8	0,01	0,07	0	3	8	0,01	0,08																				
0	1	9	**7,38**	0,23	0	3	9	**4,4**	0,2																				
0	1	10	-0,01	0,06																									
0	2	0	**166,8**	3,02																									

Space group determination by hand

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Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n* — ***F***

hkl with *h*+*k*+l = 2*n* — ***I***

hkl with *h* + *l* = 2*n* — ***B***

hkl with *k* + *l* = 2*n* — ***A***

hkl with *h* + *k* = 2*n* — ***C***

hkl all orders — ***P***

0kl with *l* = 2*n* — *Pc__*

0kl with *k* = 2*n* — *Pb__*

0kl with *k* + *l* = 2*n* — *Pn__*

0kl all orders

glide plan ⊥ b ?

h0l with *l* = 2*n* — *Pnc_*

h0l with *h* = 2*n*

h0l with *h* + *l* = 2*n*

h0l all orders

1	0	0	0,01	0,01
1	0	1	0,02	0,01
1	0	2	0,03	0,01
1	0	3	0,03	0,02
1	0	4	0,01	0,02
1	0	5	0,03	0,02
1	0	6	0,06	0,04
1	0	7	-0,07	0,04
1	0	8	-0,07	0,08
1	0	9	-0,03	0,07
1	0	10	-0,01	0,06
2	0	0	**11,03**	0,23
2	0	1	**131,3**	1,51
2	0	2	**25,39**	0,33
2	0	3	**109,5**	1,62
2	0	4	**60,83**	0,91
2	0	5	**40**	0,67
2	0	6	**5,59**	0,13
2	0	7	**2,79**	0,09
2	0	8	**1,18**	0,11
2	0	9	**3,06**	0,16
2	0	10	**8,94**	0,27
3	0	0	0,02	0,02
3	0	1	0,03	0,01
3	0	2	0,01	0,01
3	0	3	0,02	0,01
3	0	4	0,04	0,02
3	0	5	0,01	0,03
3	0	6	0	0,04
3	0	7	0,01	0,05
3	0	8	-0,01	0,07
3	0	9	0,01	0,07
3	0	10	0,07	0,06
4	0	0	**66,7**	1,49
4	0	1	**151,2**	1,69
4	0	2	**8,03**	0,12
4	0	3	**10,85**	0,17
4	0	4	**12,67**	0,21
4	0	5	**25,88**	0,44
4	0	6	**24,3**	0,43
4	0	7	**22,56**	0,33
4	0	8	**0,24**	0,08
4	0	9	**18,32**	0,4
4	0	10	**2,1**	0,11
5	0	0	0,03	0,02
5	0	1	0,01	0,01
5	0	2	0,02	0,02
5	0	3	-0,01	0,02
5	0	4	-0,02	0,02
5	0	5	-0,03	0,03
5	0	6	0,01	0,04
5	0	7	-0,03	0,05
5	0	8	0,02	0,07
5	0	9	-0,03	0,06
5	0	10	-0,11	0,06
6	0	0	**9,29**	0,22
6	0	1	**13,72**	0,2
6	0	2	**103,4**	1,4
6	0	3	**28,06**	0,41
6	0	4	**34,06**	0,53
6	0	5	**5,08**	0,13
6	0	6	**15,94**	0,33
6	0	7	**0,23**	0,07
6	0	8	**18,46**	0,38
6	0	9	**0,99**	0,09
6	0	10	**8,31**	0,24
7	0	0	0,01	0,03
7	0	1	0,01	0,02
7	0	2	0	0,02
7	0	3	0,03	0,02
7	0	4	0,01	0,03
7	0	5	0,05	0,04
7	0	6	0,03	0,04
7	0	7	-0,01	0,07
7	0	8	-0,01	0,06
7	0	9	-0,02	0,06
7	0	10	-0,05	0,05
8	0	0	**204,3**	4,1
8	0	1	**34,02**	0,53
8	0	2	**93,91**	1,51
8	0	3	**14,59**	0,25
8	0	4	**5,73**	0,13
8	0	5	**12,2**	0,26
8	0	6	**8,56**	0,18
8	0	7	**8,13**	0,24
8	0	8	**3,89**	0,14
8	0	9	**3,17**	0,11
8	0	10	**0,7**	0,07
9	0	0	0,02	0,03
9	0	1	0,04	0,03
9	0	2	-0,03	0,03
9	0	3	0,04	0,03
9	0	4	-0,01	0,04
9	0	5	-0,04	0,05
9	0	6	0,08	0,07
9	0	7	0,07	0,07
9	0	8	0,01	0,06
9	0	9	-0,01	0,05

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hkl with *h*+*k*+l = 2*n* — ***I***

hkl with *h* + *l* = 2*n* — ***B***

hkl with *k* + *l* = 2*n* — ***A***

hkl with *h* + *k* = 2*n* — ***C***

hkl all orders — ***P***

0kl with *l* = 2*n* — *Pc??*

0kl with *k* = 2*n* — *Pb??*

0kl with *k* + *l* = 2*n* — *Pn??*

0kl all orders

glide plan ⊥ b ?

h0l with *l* = 2*n* — *Pnc_*

h0l with *h* = 2*n* — *Pna_*

h0l with *h* + *l* = 2*n*

h0l all orders

1	0	0	0,01	0,01
1	0	1	0,02	0,01
1	0	2	0,03	0,01
1	0	3	0,03	0,02
1	0	4	0,01	0,02
1	0	5	0,03	0,02
1	0	6	0,06	0,04
1	0	7	-0,07	0,04
1	0	8	-0,07	0,08
1	0	9	-0,03	0,07
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2	0	4	**60,83**	0,91
2	0	5	**40**	0,67
2	0	6	**5,59**	0,13
2	0	7	**2,79**	0,09
2	0	8	**1,18**	0,11
2	0	9	**3,06**	0,16
2	0	10	**8,94**	0,27
3	0	0	0,02	0,02
3	0	1	0,03	0,01
3	0	2	0,01	0,01
3	0	3	0,02	0,01
3	0	4	0,04	0,02
3	0	5	0,01	0,03
3	0	6	0	0,04
3	0	7	0,01	0,05
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4	0	3	**10,85**	0,17
4	0	4	**12,67**	0,21
4	0	5	**25,88**	0,44
4	0	6	**24,3**	0,43
4	0	7	**22,56**	0,33
4	0	8	0,24	0,08
4	0	9	**18,32**	0,4
4	0	10	**2,1**	0,11
5	0	0	0,03	0,02
5	0	1	0,01	0,01
5	0	2	0,02	0,02
5	0	3	-0,01	0,02
5	0	4	-0,02	0,02
5	0	5	-0,03	0,03
5	0	6	0,01	0,04
5	0	7	-0,03	0,05
5	0	8	0,02	0,07
5	0	9	-0,03	0,06
5	0	10	-0,11	0,06
6	0	0	**9,29**	0,22
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6	0	3	**28,06**	0,41
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6	0	5	**5,08**	0,13
6	0	6	**15,94**	0,33
6	0	7	**0,23**	0,07
6	0	8	**18,46**	0,38
6	0	9	**0,99**	0,09
6	0	10	**8,31**	0,24
7	0	0	0,01	0,03
7	0	1	0,01	0,02
7	0	2	0	0,02
7	0	3	0,03	0,02
7	0	4	0,01	0,03
7	0	5	0,05	0,04
7	0	6	0,03	0,04
7	0	7	-0,01	0,07
7	0	8	-0,01	0,06
7	0	9	-0,02	0,06
7	0	10	-0,05	0,05
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8	0	5	**12,2**	0,26
8	0	6	**8,56**	0,18
8	0	7	**8,13**	0,24
8	0	8	**3,89**	0,14
8	0	9	**3,17**	0,11
8	0	10	**0,7**	0,07
9	0	0	0,02	0,03
9	0	1	0,04	0,03
9	0	2	-0,03	0,03
9	0	3	0,04	0,03
9	0	4	-0,01	0,04
9	0	5	-0,04	0,05
9	0	6	0,08	0,07
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9	0	9	-0,01	0,05

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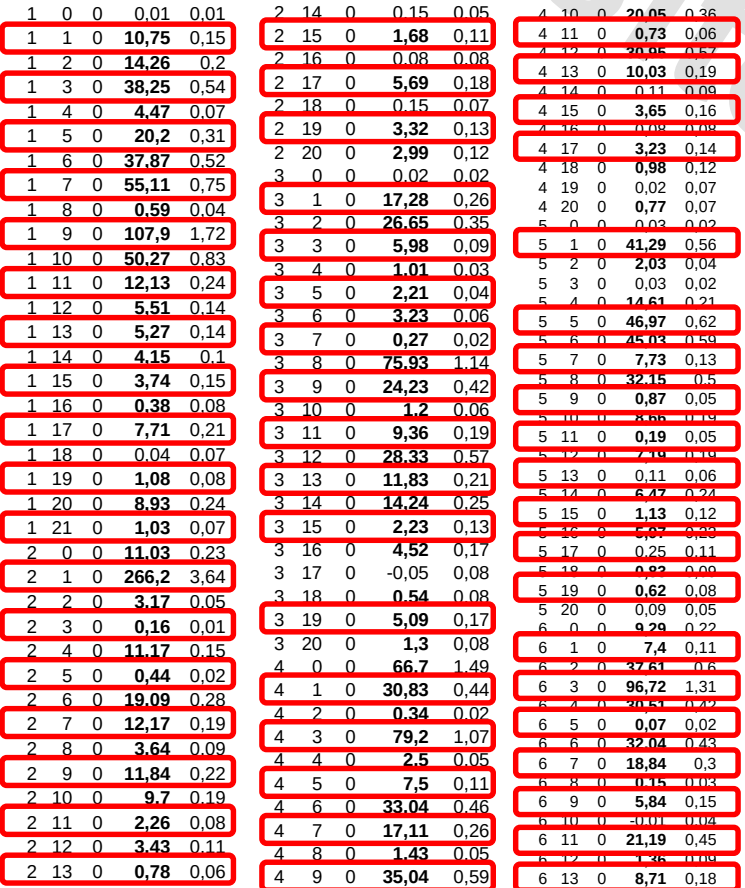
hkl with *k* + *l* = 2*n* — **A**

hkl with *h* + *k* = 2*n* — **C**

hkl all orders — **P**



h	k	l		
1	0	0	0,01	0,01
1	1	0	**10,75**	0,15
1	2	0	**14,26**	0,2
1	3	0	**38,25**	0,54
1	4	0	**4,47**	0,07
1	5	0	**20,2**	0,31
1	6	0	**37,87**	0,52
1	7	0	**55,11**	0,75
1	8	0	**0,59**	0,04
1	9	0	**107,9**	1,72
1	10	0	**50,27**	0,83
1	11	0	**12,13**	0,24
1	12	0	**5,51**	0,14
1	13	0	**5,27**	0,14
1	14	0	**4,15**	0,1
1	15	0	**3,74**	0,15
1	16	0	**0,38**	0,08
1	17	0	**7,71**	0,21
1	18	0	0,04	0,07
1	19	0	**1,08**	0,08
1	20	0	**8,93**	0,24
1	21	0	**1,03**	0,07
2	0	0	**11,03**	0,23
2	1	0	**266,2**	3,64
2	2	0	**3,17**	0,05
2	3	0	**0,16**	0,01
2	4	0	**11,17**	0,15
2	5	0	**0,44**	0,02
2	6	0	**19,09**	0,28
2	7	0	**12,17**	0,19
2	8	0	**3,64**	0,09
2	9	0	**11,84**	0,22
2	10	0	**9,7**	0,19
2	11	0	**2,26**	0,08
2	12	0	**3,43**	0,11
2	13	0	**0,78**	0,06
2	14	0	0,15	0,05
2	15	0	**1,68**	0,11
2	16	0	0,08	0,08
2	17	0	**5,69**	0,18
2	18	0	0,15	0,07
2	19	0	**3,32**	0,13
2	20	0	**2,99**	0,12
3	0	0	0,02	0,02
3	1	0	**17,28**	0,26
3	2	0	**26,65**	0,35
3	3	0	**5,98**	0,09
3	4	0	**1,01**	0,03
3	5	0	**2,21**	0,04
3	6	0	**3,23**	0,06
3	7	0	**0,27**	0,02
3	8	0	**75,93**	1,14
3	9	0	**24,23**	0,42
3	10	0	**1,2**	0,06
3	11	0	**9,36**	0,19
3	12	0	**28,33**	0,57
3	13	0	**11,83**	0,21
3	14	0	**14,24**	0,25
3	15	0	**2,23**	0,13
3	16	0	**4,52**	0,17
3	17	0	-0,05	0,08
3	18	0	**0,54**	0,08
3	19	0	**5,09**	0,17
3	20	0	**1,3**	0,08
4	0	0	**66,7**	1,49
4	1	0	**30,83**	0,44
4	2	0	**0,34**	0,02
4	3	0	**79,2**	1,07
4	4	0	**2,5**	0,05
4	5	0	**7,5**	0,11
4	6	0	**33,04**	0,46
4	7	0	**17,11**	0,26
4	8	0	**1,43**	0,05
4	9	0	**35,04**	0,59
4	10	0	**20,05**	0,36
4	11	0	**0,73**	0,06
4	12	0	**30,85**	0,57
4	13	0	**10,03**	0,19
4	14	0	0,11	0,09
4	15	0	**3,65**	0,16
4	16	0	0,08	0,08
4	17	0	**3,23**	0,14
4	18	0	**0,98**	0,12
4	19	0	0,02	0,07
4	20	0	**0,77**	0,07
5	0	0	0,03	0,02
5	1	0	**41,29**	0,56
5	2	0	**2,03**	0,04
5	3	0	0,03	0,02
5	4	0	**14,61**	0,21
5	5	0	**46,97**	0,62
5	6	0	**45,03**	0,59
5	7	0	**7,73**	0,13
5	8	0	**32,15**	0,5
5	9	0	**0,87**	0,05
5	10	0	**8,55**	0,19
5	11	0	**0,19**	0,05
5	12	0	**7,19**	0,19
5	13	0	0,11	0,06
5	14	0	**6,47**	0,24
5	15	0	**1,13**	0,12
5	16	0	**5,07**	0,23
5	17	0	0,25	0,11
5	18	0	**0,83**	0,09
5	19	0	**0,62**	0,08
5	20	0	0,09	0,05
6	0	0	**9,29**	0,22
6	1	0	**7,4**	0,11
6	2	0	**37,61**	0,6
6	3	0	**96,72**	1,31
6	4	0	**30,51**	0,42
6	5	0	**0,07**	0,02
6	6	0	**32,04**	0,43
6	7	0	**18,84**	0,3
6	8	0	**0,15**	0,03
6	9	0	**5,84**	0,15
6	10	0	-0,01	0,04
6	11	0	**21,19**	0,45
6	12	0	**1,36**	0,08
6	13	0	**8,71**	0,18

0kl with *l* = 2*n* — *Pc??*

0kl with *k* = 2*n* — *Pb??*

0kl with *k* + *l* = 2*n* — *Pn??*

0kl all orders

glide plan ⊥ b ?

h0l with *l* = 2*n* — *Pnc_*

h0l with *h* = 2*n* — *Pna_*

h0l with *h* + *l* = 2*n*

h0l all orders

glide plan ⊥ c ?

hk0 with *k* = 2*n* — *Pnab*

hk0 with *h* = 2*n*

hk0 with *h*+*k* = 2*n*

hk0 all orders

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, *b* = 17.4848(3) Å, *c* = 8.9597(2) Å, **α = 90°**, **β = 90°**, **γ = 90°**

Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n*	hkl with *h*+*k*+l = 2*n*	hkl with *h* + *l* = 2*n*	hkl with *k* + *l* = 2*n*	hkl with *h* + *k* = 2*n*	hkl all orders
F	***I***	***B***	***A***	***C***	***P***

1	0	0	0,01	0,01
1	1	0	**10,75**	0,15
1	2	0	**14,26**	0,2
1	3	0	**38,25**	0,54
1	4	0	**4,47**	0,07
1	5	0	**20,2**	0,31
1	6	0	**37,87**	0,52
1	7	0	**55,11**	0,75
1	8	0	**0,59**	0,04
1	9	0	**107,9**	1,72
1	10	0	**50,27**	0,83
1	11	0	**12,13**	0,24
1	12	0	**5,51**	0,14
1	13	0	**5,27**	0,14
1	14	0	**4,15**	0,1
1	15	0	**3,74**	0,15
1	16	0	**0,38**	0,08
1	17	0	**7,71**	0,21
1	18	0	0,04	0,07
1	19	0	**1,08**	0,08
1	20	0	**8,93**	0,24
1	21	0	**1,03**	0,07
2	0	0	**11,03**	0,23
2	1	0	**266,2**	3,64
2	2	0	**3,17**	0,05
2	3	0	**0,16**	0,01
2	4	0	**11,17**	0,15
2	5	0	**0,44**	0,02
2	6	0	**19,09**	0,28
2	7	0	**12,17**	0,19
2	8	0	**3,64**	0,09
2	9	0	**11,84**	0,22
2	10	0	**9,7**	0,19
2	11	0	**2,26**	0,08
2	12	0	**3,43**	0,11
2	13	0	**0,78**	0,06

2	14	0	0,15	0,05
2	15	0	**1,68**	0,11
2	16	0	0,08	0,08
2	17	0	**5,69**	0,18
2	18	0	0,15	0,07
2	19	0	**3,32**	0,13
2	20	0	**2,09**	0,12
3	0	0	0,02	0,02
3	1	0	**17,28**	0,26
3	2	0	**26,65**	0,35
3	3	0	**5,98**	0,09
3	4	0	**1,01**	0,03
3	5	0	**2,21**	0,04
3	6	0	**3,23**	0,06
3	7	0	**0,27**	0,02
3	8	0	**75,93**	1,14
3	9	0	**24,23**	0,42
3	10	0	**1,2**	0,06
3	11	0	**9,36**	0,19
3	12	0	**28,33**	0,57
3	13	0	**11,83**	0,21
3	14	0	**14,24**	0,25
3	15	0	**2,23**	0,13
3	16	0	**4,52**	0,17
3	17	0	-0,05	0,08
3	18	0	**0,54**	0,08
3	19	0	**5,09**	0,17
3	20	0	**1,3**	0,08
4	0	0	**66,7**	1,49
4	1	0	**30,83**	0,44
4	2	0	**0,34**	0,02
4	3	0	**79,2**	1,07
4	4	0	**2,5**	0,05
4	5	0	**7,5**	0,11
4	6	0	**33,04**	0,46
4	7	0	**17,11**	0,26
4	8	0	**1,43**	0,05
4	9	0	**35,04**	0,59

4	10	0	**20,05**	0,36
4	11	0	**0,73**	0,06
4	12	0	**30,95**	0,57
4	13	0	**10,03**	0,19
4	14	0	0,11	0,09
4	15	0	**3,65**	0,16
4	16	0	0,08	0,08
4	17	0	**3,23**	0,14
4	18	0	**0,98**	0,12
4	19	0	0,02	0,07
4	20	0	**0,77**	0,07
5	0	0	0,03	0,02
5	1	0	**41,29**	0,56
5	2	0	**2,03**	0,04
5	3	0	0,03	0,02
5	4	0	**14,61**	0,21
5	5	0	**46,97**	0,62
5	6	0	**45,03**	0,59
5	7	0	**7,73**	0,13
5	8	0	**32,15**	0,5
5	9	0	**0,87**	0,05
5	10	0	**8,66**	0,19
5	11	0	**0,19**	0,05
5	12	0	**7,19**	0,19
5	13	0	0,11	0,06
5	14	0	**6,47**	0,24
5	15	0	**1,13**	0,12
5	16	0	**5,97**	0,23
5	17	0	0,25	0,11
5	18	0	**0,83**	0,09
5	19	0	**0,62**	0,08
5	20	0	0,09	0,05
6	0	0	**9,29**	0,22
6	1	0	**7,4**	0,11
6	2	0	**37,61**	0,6
6	3	0	**96,72**	1,31
6	4	0	**30,51**	0,42
6	5	0	**0,07**	0,02
6	6	0	**32,04**	0,43
6	7	0	**18,84**	0,3
6	8	0	**0,15**	0,03
6	9	0	**5,84**	0,15
6	10	0	-0,01	0,04
6	11	0	**21,19**	0,45
6	12	0	**1,36**	0,09
6	13	0	**8,71**	0,18

0kl with *l* = 2*n*	0kl with *k* = 2*n*	0kl with *k* + *l* = 2*n*	0kl all orders
Pc??	*Pb??*	*Pn??*	

glide plan ⊥ b ?

h0l with *l* = 2*n*	h0l with *h* = 2*n*	h0l with *h* + *l* = 2*n*	h0l all orders
*Pnc_*	*Pna_*		

glide plan ⊥ c ?

hk0 with *k* = 2*n*	hk0 with *h* = 2*n*	hk0 with *h*+*k* = 2*n*	hk0 all orders
Pnab	*Pnaa*		

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, *b* = 17.4848(3) Å, *c* = 8.9597(2) Å, **α = 90°**, **β = 90°**, **γ = 90°**

Test for centering

hkl with *h* + *k* = 2*n* and *k* + *l* = 2*n* — ***F***

hkl with *h*+*k*+l = 2*n* — ***I***

hkl with *h* + *l* = 2*n* — ***B***

hkl with *k* + *l* = 2*n* — ***A***

hkl with *h* + *k* = 2*n* — ***C***

hkl all orders — ***P***

1	0	0	0,01	0,01	2	14	0	0,15	0,05	4	10	0	**20,05**	0,36
1	1	0	**10,75**	0,15	2	15	0	**1,68**	0,11	4	11	0	**0,73**	0,06
1	2	0	**14,26**	0,2	2	16	0	0,08	0,08	4	12	0	**30,85**	0,57
1	3	0	**38,25**	0,54	2	17	0	**5,69**	0,18	4	13	0	**10,03**	0,19
1	4	0	**4,47**	0,07	2	18	0	0,15	0,07	4	14	0	0,11	0,09
1	5	0	**20,2**	0,31	2	19	0	**3,32**	0,13	4	15	0	**3,65**	0,16
1	6	0	**37,87**	0,52	2	20	0	**2,99**	0,12	4	16	0	0,08	0,08
1	7	0	**55,11**	0,75	3	0	0	0,02	0,02	4	17	0	**3,23**	0,14
1	8	0	**0,59**	0,04	3	1	0	**17,28**	0,26	4	18	0	**0,98**	0,12
1	9	0	**107,9**	1,72	3	2	0	**26,65**	0,35	4	19	0	0,02	0,07
1	10	0	**50,27**	0,83	3	3	0	**5,98**	0,09	4	20	0	**0,77**	0,07
1	11	0	**12,13**	0,24	3	4	0	**1,01**	0,03	5	0	0	0,03	0,02
1	12	0	**5,51**	0,14	3	5	0	**2,21**	0,04	5	1	0	**41,29**	0,56
1	13	0	**5,27**	0,14	3	6	0	**3,23**	0,06	5	2	0	**2,03**	0,04
1	14	0	**4,15**	0,1	3	7	0	**0,27**	0,02	5	3	0	0,03	0,02
1	15	0	**3,74**	0,15	3	8	0	**75,93**	1,14	5	4	0	**14,61**	0,21
1	16	0	**0,38**	0,08	3	9	0	**24,23**	0,42	5	5	0	**46,97**	0,62
1	17	0	**7,71**	0,21	3	10	0	**1,2**	0,06	5	6	0	**45,03**	0,59
1	18	0	0,04	0,07	3	11	0	**9,36**	0,19	5	7	0	**7,73**	0,13
1	19	0	**1,08**	0,08	3	12	0	**28,33**	0,57	5	8	0	**32,15**	0,5
1	20	0	**8,93**	0,24	3	13	0	**11,83**	0,21	5	9	0	**0,87**	0,05
1	21	0	**1,03**	0,07	3	14	0	**14,24**	0,25	5	10	0	**8,66**	0,19
2	0	0	**11,03**	0,23	3	15	0	**2,23**	0,13	5	11	0	**0,19**	0,05
2	1	0	**266,2**	3,64	3	16	0	**4,52**	0,17	5	12	0	**7,19**	0,19
2	2	0	**3,17**	0,05	3	17	0	-0,05	0,08	5	13	0	**0,11**	0,06
2	3	0	**0,16**	0,01	3	18	0	**0,54**	0,08	5	14	0	**6,47**	0,24
2	4	0	**11,17**	0,15	3	19	0	**5,09**	0,17	5	15	0	**1,13**	0,12
2	5	0	**0,44**	0,02	3	20	0	**1,3**	0,08	5	16	0	**5,97**	0,23
2	6	0	**19,09**	0,28	4	0	0	**66,7**	1,49	5	17	0	**0,25**	0,11
2	7	0	**12,17**	0,19	4	1	0	**30,83**	0,44	5	18	0	**0,83**	0,09
2	8	0	**3,64**	0,09	4	2	0	**0,34**	0,02	5	19	0	**0,62**	0,08
2	9	0	**11,84**	0,22	4	3	0	**79,2**	1,07	5	20	0	0,09	0,05
2	10	0	**9,7**	0,19	4	4	0	**2,5**	0,05	6	0	0	**9,29**	0,22
2	11	0	**2,26**	0,08	4	5	0	**7,5**	0,11	6	1	0	**7,4**	0,11
2	12	0	**3,43**	0,11	4	6	0	**33,04**	0,46	6	2	0	**37,61**	0,6
2	13	0	**0,78**	0,06	4	7	0	**17,11**	0,26	6	3	0	**96,72**	1,31
					4	8	0	**1,43**	0,05	6	4	0	**30,51**	0,42
					4	9	0	**35,04**	0,59	6	5	0	**0,07**	0,02
										6	6	0	**32,04**	0,43
										6	7	0	**18,84**	0,3
										6	8	0	**0,15**	0,03
										6	9	0	**5,84**	0,15
										6	10	0	-0,01	0,04
										6	11	0	**21,19**	0,45
										6	12	0	**1,36**	0,09
										6	13	0	**8,71**	0,18

0kl with *l* = 2*n* — *Pc??*

0kl with *k* = 2*n* — *Pb??*

0kl with *k* + *l* = 2*n* — *Pn??*

0kl all orders

glide plan ⊥ b ?

h0l with *l* = 2*n* — *Pnc_*

h0l with *h* = 2*n* — *Pna_*

h0l with *h* + *l* = 2*n*

h0l all orders

glide plan ⊥ c ?

hk0 with *k* = 2*n* — *Pnab*

hk0 with *h* = 2*n* — *Pnaa*

hk0 with *h*+*k* = 2*n* — *Pnaa*

hk0 all orders

Space group determination by hand

Example Paul32:

a = 18.4398(3) Å, b = 17.4848(3) Å, c = 8.9597(2) Å, **$\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$**

Test for centering

hkl with $h + k = 2n$ and $k + l = 2n$	hkl with $h+k+l = 2n$	hkl with $h + l = 2n$	hkl with $k + l = 2n$	hkl with $h + k = 2n$	hkl all orders
F	***I***	***B***	***A***	***C***	***P***

glide plan ⊥ a ?

0kl with $l = 2n$	0kl with $k = 2n$	0kl with $k + l = 2n$	0kl all orders
Pc??	*Pb??*	*Pn??*	

glide plan ⊥ b ?

h0l with $l = 2n$	h0l with $h = 2n$	h0l with $h + l = 2n$	h0l all orders
*Pnc_*	*Pna_*		

glide plan ⊥ c ?

hk0 with $k = 2n$	hk0 with $h = 2n$	hk0 with $h+k = 2n$	hk0 all orders
Pnab	*Pnaa*	*Pnaa*	*Pnam* *Pna2$_1$*

Why can we not differentiate between *Pnam* and *Pna*2_1 with the reflection conditions for a 2_1-axis $\parallel c$?

Reflection condition:

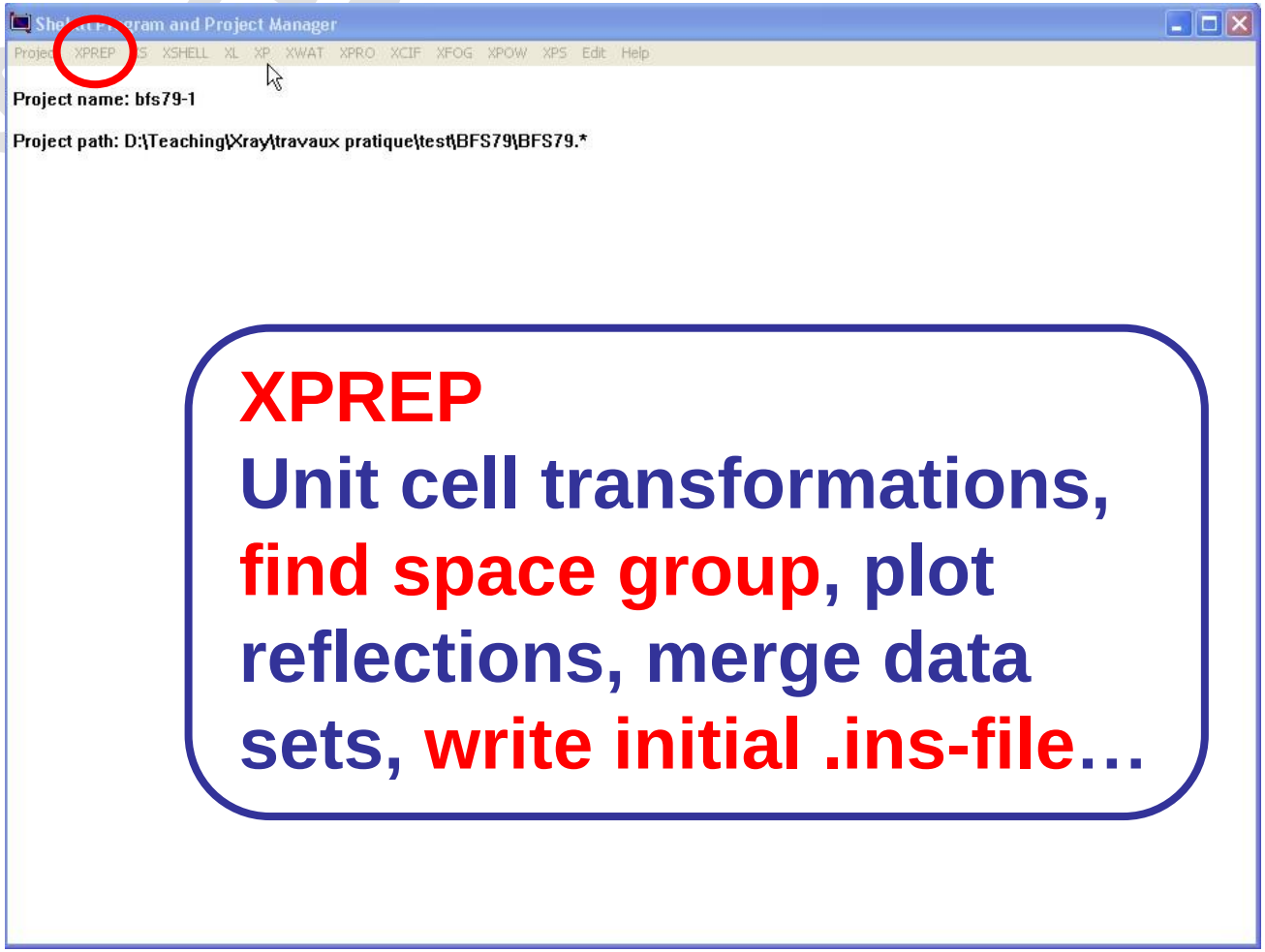
$2_1 \parallel c$: 00l with $l = 2n$

But: 0kl with $k + l = 2n$ due to $n \perp a$, thus 00l with $l = 2n$ always respected.

Systematic absences in XPREP

- Determination which screw axes and glide planes are present.
- Determination which space groups contain these symmetry elements.

- By hand
- With XPREP

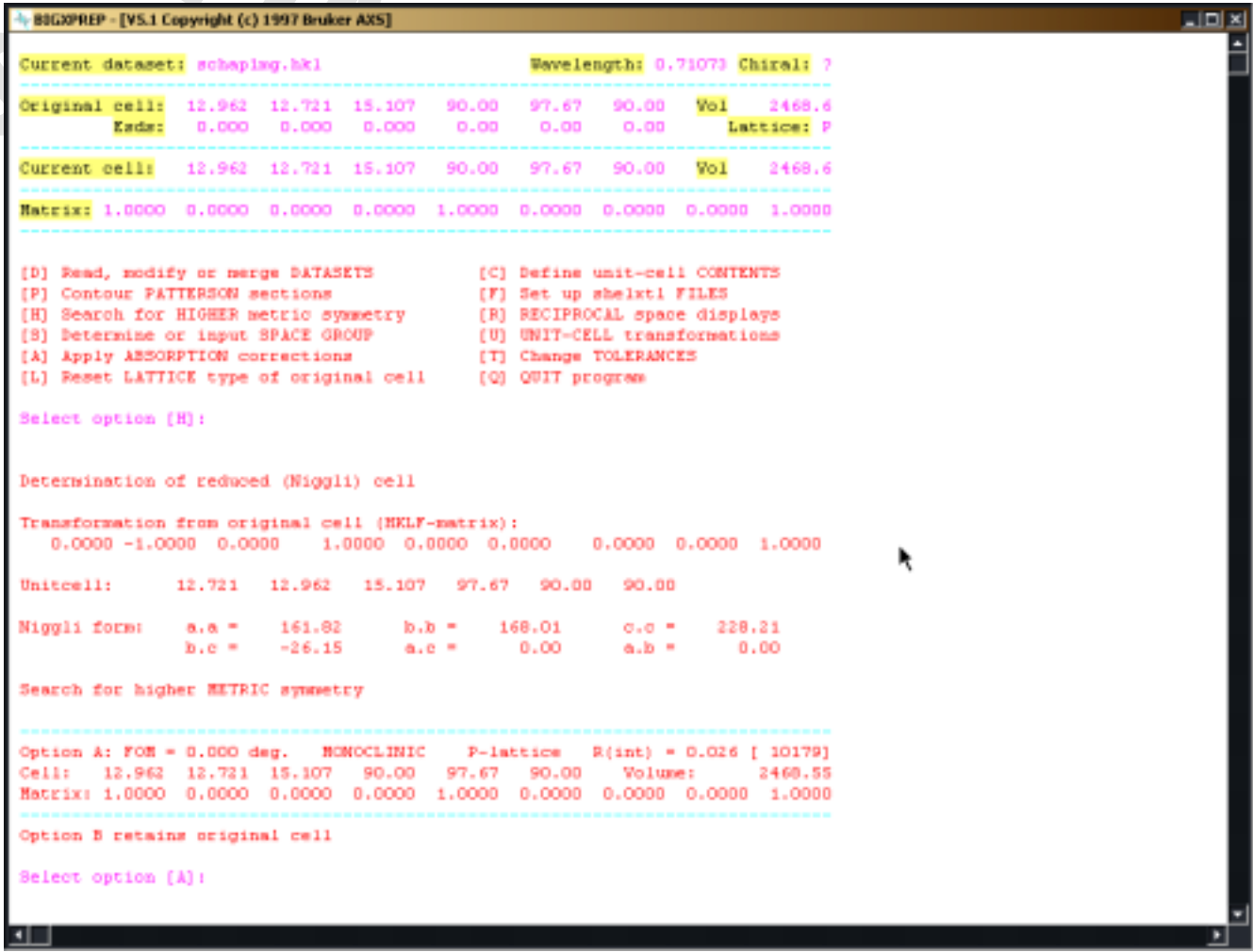


Space group determination with XPREP

Determination of the possible Bravais lattice: Often already done by a previous program

Reduced (Niggli) cell
Primitive unit cell with a < b < c and all angles either >/= 90° or </= 90°. For any crystal there is only **one** cell which fulfills these conditions. The reduced cell is useful to compare unit cells, since it is independent from user choices.

Unit cells the program finds acceptable.



Space group determination with XPREP

Unit cell employed by the program(s)

Original unit cell

Confirmation of the Bravais lattice:

Crystal system

Centering

```
BIGXPREP - [V5.1 Copyright (c) 1997 Bruker AXS]

Current dataset: schap1mg.hkl                    Wavelength: 0.71073 Chiral: ?
-------------------------------------------------------------------------------
Original cell:  12.962  12.721  15.107  90.00   97.67   90.00   Vol    2468.6
          Esds:  0.000   0.000   0.000   0.00    0.00    0.00      Lattice: P
-------------------------------------------------------------------------------
Current cell:   12.962  12.721  15.107  90.00   97.67   90.00   Vol    2468.6
-------------------------------------------------------------------------------
Matrix: 1.0000  0.0000  0.0000  0.0000  1.0000  0.0000  0.0000  0.0000  1.0000
-------------------------------------------------------------------------------
Crystal system: Monoclinic              Lattice: P
-------------------------------------------------------------------------------

[S] Determine SPACE GROUP
[C] Must be CHIRAL (sample is optically active)
[N] NOT NECESSARILY chiral (eg. may be racemate)
[I] INPUT known space group
[E] EXIT to main menu  or  [Q] QUIT program

Select option [S]:


[A] Triclinic,  [M] Monoclinic,  [O] Orthorhombic,  [T] Tetragonal,
[H] Trigonal/Hexagonal,  [C] Cubic  or  [E] EXIT

Select option [M]:


Lattice exceptions: P      A      B      C      I      F      Obv    Rev    All

N (total) =          0   7643   7646   7629   7643  11459  10187  10175  15264
N (int>3sigma) =     0   5858   5714   5868   5885   8720   7755   7760  11691
Mean intensity =   0.0   22.2   21.4   21.5   20.7   21.7   22.3   21.9   22.0
Mean int/sigma =   0.0   20.2   19.8   19.9   19.8   20.0   20.2   20.2   20.1

Lattice type [P, A, B, C, I, F, O(obv.), R(rev. rhomb. on hex. axes)]

Select option [P]:
```

Space group determination with XPREP

Reflections which **violate** the reflection condition. For **A** centering: k + l = 2n

Of the reflections above, those with **non-zero intensity**

Lattice exceptions:	P	A	B	C	I	F	Obv	Rev	All
N (total) =	0	7643	7646	7629	7643	11459	10187	10175	15264
N (int>3sigma) =	0	5858	5714	5868	5885	8720	7755	7760	11691
Mean intensity =	0.0	22.2	21.4	21.5	20.7	21.7	22.3	21.9	22.0
Mean int/sigma =	0.0	20.2	19.8	19.9	19.8	20.0	20.2	20.2	20.1

There are no reflection conditions for a primitive cell

Compare to the values for all reflections

Average intensity and signal noise ratio for these reflections

If we would have A centering:

	A
	7643
	858
	1.3
	0.2

Space group determination with XPREP

Determination of the space group using systematic absences

Systematic absence exceptions:

	-21-	-a-	-c-	-n-
N	16	369	364	371
N I>3s	0	168	169	11
<I>	0.1	32.0	32.5	0.1
<I/s>	0.8	18.3	18.7	0.8

Systematic absences

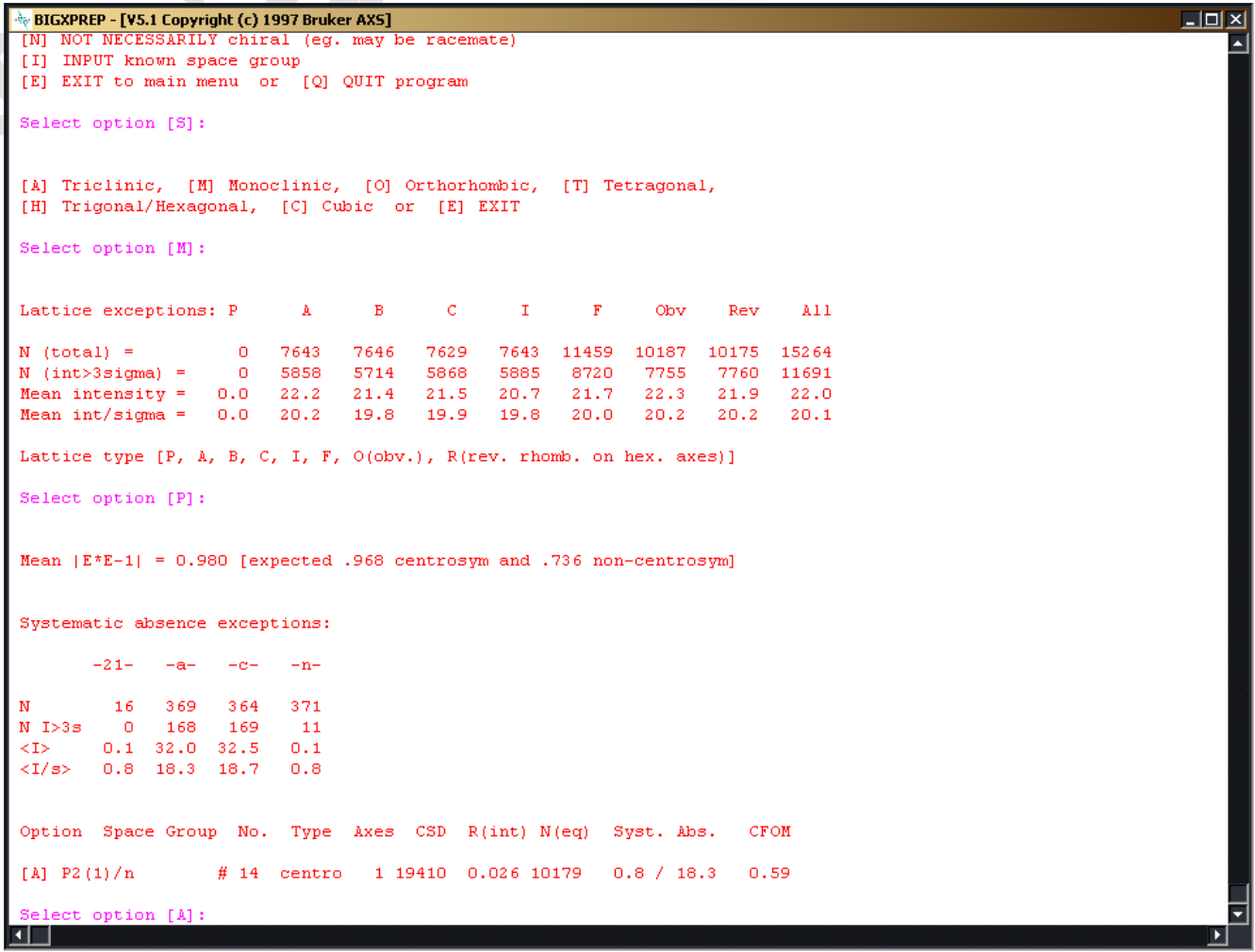
```
\XS]
ay be racemate)

IT program

[O] Orthorhombic,  [T] Tetragonal,
c  or  [E] EXIT

 B      C      I      F      Obv    Rev    All
646   7629   7643  11459  10187  10175  15264
714   5868   5885   8720   7755   7760  11691
1.4   21.5   20.7   21.7   22.3   21.9   22.0
9.8   19.9   19.8   20.0   20.2   20.2   20.1

(obv.), R(rev. rhomb. on hex. axes)]

Mean |E*E-1| = 0.980 [expected .968 centrosym and .736 non-centrosym]

Systematic absence exceptions:

      -21-   -a-   -c-   -n-

N       16   369   364   371
N I>3s   0   168   169    11
<I>    0.1  32.0  32.5   0.1
<I/s>  0.8  18.3  18.7   0.8

Option  Space Group  No.  Type  Axes  CSD  R(int) N(eq)  Syst. Abs.   CFOM

[A] P2(1)/n        # 14  centro   1 19410  0.026 10179   0.8 / 18.3   0.59

Select option [A]:
```

Again, compare with the values for all reflections

Space group determination with XPREP

Determination of the space group using systematic absences

E-statistics



```
BIGXPREP - [V5.1 Copyright (c) 1997 Bruker AXS]
[N] NOT NECESSARILY chiral (eg. may be racemate)
[I] INPUT known space group
[E] EXIT to main menu  or  [Q] QUIT program

Select option [S]:


[A] Triclinic,  [M] Monoclinic,  [O] Orthorhombic,  [T] Tetragonal,
[H] Trigonal/Hexagonal,  [C] Cubic  or  [E] EXIT

Select option [M]:


Lattice exceptions: P      A      B      C      I      F      Obv    Rev    All

N (total) =          0   7643   7646   7629   7643  11459  10187  10175  15264
N (int>3sigma) =     0   5858   5714   5868   5885   8720   7755   7760  11691
Mean intensity =   0.0   22.2   21.4   21.5   20.7   21.7   22.3   21.9   22.0
Mean int/sigma =   0.0   20.2   19.8   19.9   19.8   20.0   20.2   20.2   20.1

Lattice type [P, A, B, C, I, F, O(obv.), R(rev. rhomb. on hex. axes)]

Select option [P]:


Mean |E*E-1| = 0.980 [expected .968 centrosym and .736 non-centrosym]


Systematic absence exceptions:

       -21-   -a-   -c-   -n-

N        16   369   364   371
N I>3s    0   168   169    11
<I>     0.1  32.0  32.5   0.1
<I/s>   0.8  18.3  18.7   0.8


Option  Space Group  No.  Type  Axes  CSD  R(int) N(eq)  Syst. Abs.   CFOM

[A] P2(1)/n        # 14  centro   1 19410  0.026 10179   0.8 / 18.3   0.59

Select option [A]:
```

Statistical evidence for an inversion center

The theoretical distribution of intensities is different for centrosymmetric and non-centrosymmetric structures.

Since the intensities depend on the reflection angle θ, we use **normalized structure factors E**.

$$E_{hkl}^2 = I_{hkl} \Big/ \langle I_{hkl} \rangle_\theta$$

Centrosymmetric:

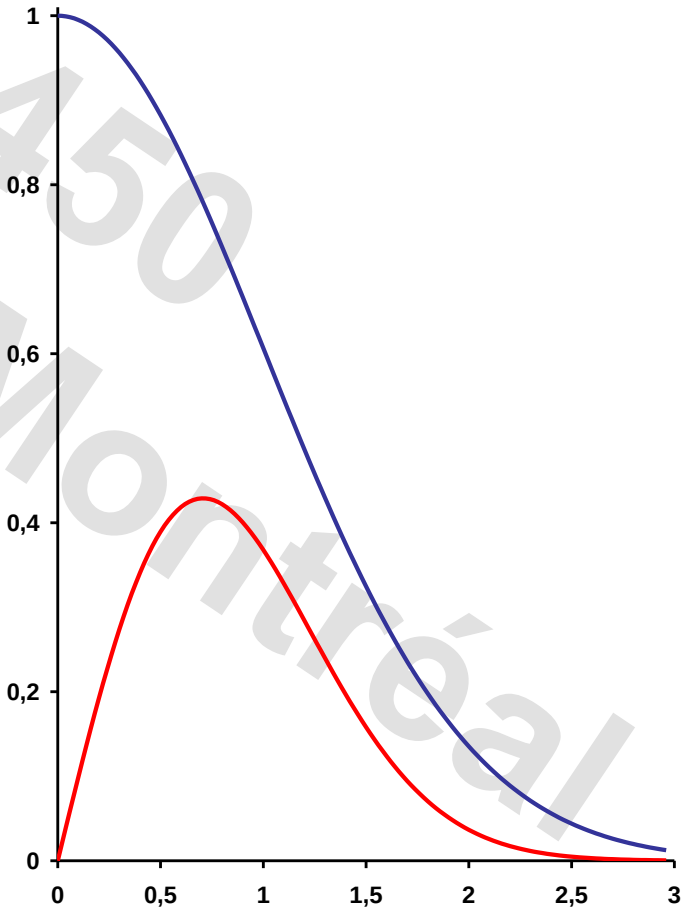
Greater probability for strong or weak reflections

$$P(E) = e^{-\frac{1}{2}|E|^2}$$

Non-centrosymmetric:

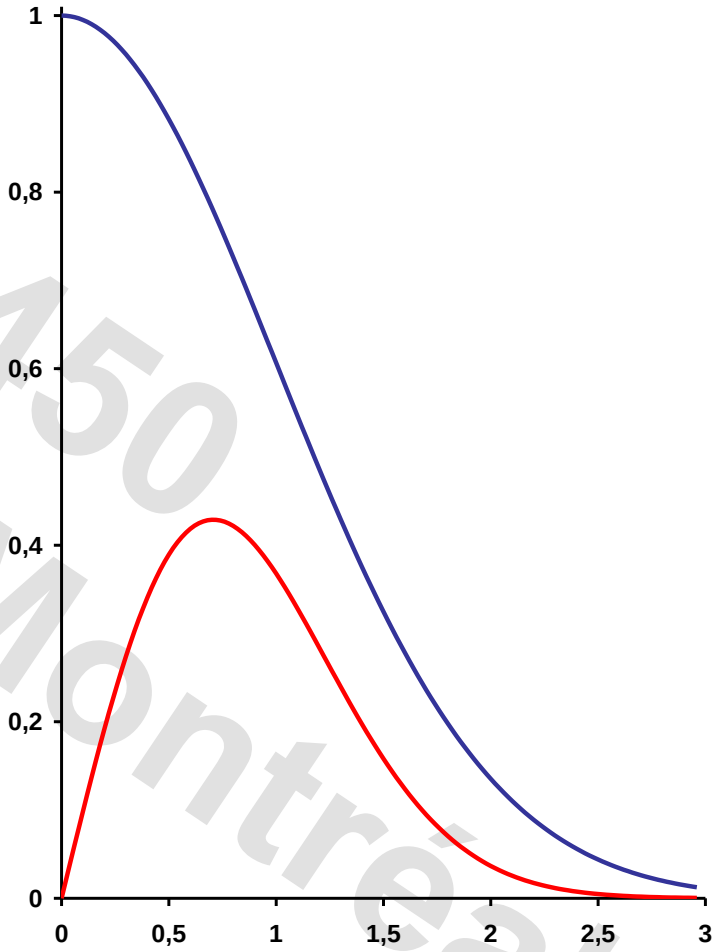
Distribution around an average value

$$P(E) = |E| e^{-|E|^2}$$



E statistics

	centrosym.	non-centrosym.
	$P(E) = e^{-\frac{1}{2}\lvert E\rvert^2}$	$P(E) = \lvert E\rvert e^{-\lvert E\rvert^2}$
$\lvert E\rvert < 1$	63.1%	61.4%
$\lvert E\rvert > 1$	31.7%	36.8%
$\lvert E\rvert > 2$	4.6%	1.8%
$\lvert E\rvert > 3$	0.3%	0.01%
$\langle\lvert E\rvert^2\rangle$	1.000	1.000
$\langle\lvert E^2-1\rvert\rangle$	0.968	0.736
$\langle\lvert E\rvert\rangle$	0.798	0.886



E statistics

	centrosym.	non-centrosym.
$\langle\lvert E^2-1\rvert\rangle$	0.968	0.736

- Real structures do not have a uniform distribution of atoms and the values might differ from the theoretical ones.
- **0.74-0.97:** A non-centrosymmetric structure easily can have tendencies towards centrosymmetry, without fulfilling it completely. A value of 0.85 indicates thus more likely a non-centrosymmetric than a centrosymmetric space group.
- **«0.74:** A value notably smaller than 0.74 might indicate twinning.
- **»0.97:** A value much higher than 0.97 might indicate "hypersymmetry": The asymmetric unit of a centrosymmetric structure is nearly centrosymmetric itself.

Space group determination with XPREP

Determination of the space group using systematic absences

```
Option  Space Group  No.  Type  Axes  CSD  R(int) N(eq)  Syst. Abs.  CFOM

[A] P2(1)/n        # 14  centro   1 19410  0.026 10179  0.8 / 18.3  0.59

Select option [A]:
```

If several space groups seem possible, you have to try all of them!

We will deal with problems here later.

Acceptable space groups

```
[H] Trigonal/Hexagonal,  [C] Cubic  or  [E] EXIT

Select option [M]:


Lattice exceptions: P      A      B      C      I      F     Obv    Rev    All

N (total) =          0   7643   7646   7629   7643  11459  10187  10175  15264
N (int>3sigma) =     0   5858   5714   5868   5885   8720   7755   7760  11691
Mean intensity =   0.0   22.2   21.4   21.5   20.7   21.7   22.3   21.9   22.0
Mean int/sigma =   0.0   20.2   19.8   19.9   19.8   20.0   20.2   20.2   20.1

Lattice type [P, A, B, C, I, F, O(obv.), R(rev. rhomb. on hex. axes)]

Select option [P]:


Mean |E*E-1| = 0.980 [expected .968 centrosym and .736 non-centrosym]


Systematic absence exceptions:

       -21-   -a-   -c-   -n-

N         16   369   364   371
N I>3s     0   168   169    11
<I>      0.1  32.0  32.5   0.1
<I/s>    0.8  18.3  18.7   0.8


Option  Space Group  No.  Type  Axes  CSD  R(int) N(eq)  Syst. Abs.  CFOM

[A] P2(1)/n        # 14  centro   1 19410  0.026 10179  0.8 / 18.3  0.59

Select option [A]:
```

Ambiguities in space group determination

36770 reflections read from file paul32.hkl Mean I/sig(I) = 10.55

Lattice exceptions	P	A	B	C	I	F	Obv	Rev	All
Total no. reflections	0	18455	18302	18397	18426	27577	24453	24449	36770
Total with I>3sig(I)	0	14415	14946	14937	14677	22149	19920	19917	30028
Mean I/sig(I) (all)	0.0	10.1	10.5	10.5	10.3	10.3	10.5	10.5	**10.5**
Mean I/sig(I) I>3sig(I)	0.0	12.6	12.6	12.7	12.7	12.6	12.6	12.6	**12.6**

Suggested lattice type is P

R(int) values for merging under all Laue symmetries :

Laue class	R(int)	N(obs)	N(ind)	R1	<n>
-1	0.039	36552	10109	0.045	3.616
2/m	0.043	36746	5469	0.046	6.719
mmm	**0.044**	**36764**	**3022**	**0.046**	**12.165**
4/m	0.563	36760	2924	0.582	12.572
4/mmm	0.566	36768	1633	0.577	22.516
-3(rhomb)	0.700	36645	5389	0.731	6.800
-3m(rhomb)	0.803	36735	3112	0.823	11.804
-3(hex)	0.720	36689	5228	0.749	7.018
-3m1(hex)	0.804	36748	2911	0.825	12.624
-31m(hex)	0.806	36746	2855	0.825	12.871
6/m	0.729	36759	2835	0.745	12.966
6/mmm	0.809	36767	1632	0.821	22.529
m-3	0.710	36767	1630	0.720	22.556
m-3m	0.811	36769	951	0.818	38.664
2/m 1 1	0.042	36748	5462	0.045	6.728
1 1 2/m	0.043	36739	5628	0.046	6.528

Highest diffraction symmetry with reasonable value of R(int) is mmm

Highest diffraction symmetry compatible with the cell metrics is mmm

Group	Cond.	Op.	All	Odd	Cut1	Cut2	Cut3	<I/sI>	Op.	No.
h00	h=2n+1		92	47	0	0	0	0.0	21..	1
0k0	k=2n+1		96	48	0	0	0	0.0	.21.	2
00l	l=2n+1		39	23	0	0	0	0.0	..21	3
0kl	k=2n+1	b..	1395	718	269	238	179	6.0		4
0kl	l=2n+1	c..		702	269	238	179	6.2		5
0kl	**k+l=2n+1**			**710**	**0**	**0**	**0**	**0.0**	**n..**	**6**
h0l	**h=2n+1**		**1441**	**734**	**0**	**0**	**0**	**0.0**	**.a.**	**7**
h0l	l=2n+1	.c.		736	279	239	192	6.0		8
h0l	h+l=2n+1	.n.		708	279	239	192	6.3		9
hk0	h=2n+1	..a	2663	1321	707	487	296	6.7		10
hk0	k=2n+1	..b		1327	650	479	290	6.5		11
hk0	h+k=2n+1	..n		1330	665	486	280	6.4		12
hkl	k+l=2n+1	A..		18432	8906	5822	3328	5.7		13
hkl	h+l=2n+1	.B.		18279	9231	5983	3491	6.1		14
hkl	h+k=2n+1	..C		18397	9395	6215	3385	6.0		15
hkl	h+k+l=2n+1	I		18403	9222	6264	3465	6.0		16
hkl	not all odd/even	F		27554	13766	9010	5102	5.9		17
h00	h=4n+1	41..		73	17	17	5	3.1		18
0k0	k=4n+1	.41.		74	26	16	9	3.9		19
00l	l=4n+1	..41		33	8	8	8	5.4		20
0kl	k+l=4n+1	d..		1045	259	215	149	3.6		21
h0l	h+l=4n+1	.d.		1074	403	356	253	5.8		22
hk0	h+k=4n+1	..d		1976	1011	722	422	6.5		23

Candidate space groups (NS = non-standard setting) :

H-M symbol		No.	Centric	Laue class	M	R(int)	N(obs)	CSD	ICSD	CFOM
P n a 21		33	no	mmm	4	0.044	36764	3013	313	**4.399**
P n a m	NS	62	yes	mmm	8	0.044	36764	3005	2296	**4.399**

The program cannot distinguish between these two space groups. A proposition will be made (often) from E-statistics and general frequency of occurrence.