

Macromolecular Crystallography School

MCS2016 25 - 29 May 2016

Dear student,

To allow you to obtain the maximum profit from the School you are invited to study, before attending the School, the first 12 pages of Fundamental of Crystallography, by Oxford University Press, ed. by C. Giacovazzo, ed. 3. These pages can be downloaded at your convenience from:

<http://www.xtal.iqfr.csic.es/MCS2016/Book-Carmelo-Giacovazzo.pdf>

It will be assumed, for teaching economy, that any student perfectly knows the scientific content of such pages: in particular he/she should dominate the meaning and the notation of the crystallographic symmetry operators. In absence of this information, it will be very difficult to understand the crystallographic symmetry in direct and reciprocal space, and the student will probably be unable to correctly make the exercises individually assigned during the School.

Once these 12 pages have been studied, please check your expertise by answering the following exercises. If you are unable to answer some of them, please return to study the text of the released pages.

If you have still difficulties, you can contact the tutor at carmelo.giacovazzo@ic.cnr.it . He will be pleased to help you.

The organizers

Armando Albert
Juan A. Hermoso
Isabel Usón

The tutor

Carmelo Giacovazzo

PS. This document, containing the questions shown below, can also be downloaded from:

<http://www.xtal.iqfr.csic.es/MCS2016/MCS2016-questions.pdf>

Macromolecular Crystallography School

MCS2016 25 - 29 May 2016

Questions and exercises for homework

- 1) If an operator 4_1 exists, should you find a 2_1 operator along the same direction?
- 2) If an operator -6 exist, should you find a mirror m perpendicular to the -6 direction?
- 3) How should you orient your hands to simulate a -1 ?
- 4) How should you orient your hands to simulate a -4 ? Does -4 implies an inversion centre?
- 5) Are you able to provide a definition for the symmetry axis n and for the symmetry axis $-n$?
- 6) Can you orient your hands to simulate a twofold axis?
- 7) Can you suitably orient two enantiomeric molecules in such a way that they are related by a twofold axis?
- 8) Please derive the equivalent positions drawn in Fig.1.3 of Fundamentals, by using the same international notation.
- 9) Can you define what a lattice represents?
- 10) Can you define what a lattice point represents?
- 11) Are the coordinates of the lattice points always integer numbers?
- 12) When you fix the origin of a direct lattice, are you obliged to locate the origin lattice point on an atom?
- 13) Can you find a centered unit cell smaller than a primitive?
- 14) How do you express a crystallographic direction?
- 15) To which direction the symbol $[132]$ corresponds? Are you able to draw such direction?
- 16) Do the crystallographic directions exhaust all the possible directions?
- 17) Are you able to draw the family of crystallographic planes $(2\ 6\ 3)$?
- 18) Which is the difference between the families (hkl) and $(-h\ -k\ -l)$?
- 19) Can you tile your room by regular pentagonal or octagonal tiles?
- 20) In the crystals is the symmetry operator 4_1 different from 4_5 ?
- 21) Does the glide plane of type b perpendicular to the b axis exist?
- 22) Which are the symmetry restrictions fixed by the periodic nature of the crystals to the order of the symmetry operators?
- 23) Which are the symmetry restrictions fixed by the periodic nature of the crystals to the translational components of the symmetry operators?

Macromolecular Crystallography School

MCS2016 25 - 29 May 2016

- 24) In crystallography, do you need the screw axis 4_6 ? Is it different from 4_2 ?
- 25) Are you able to represent, as in Fig. 1.3 of Fundamentals, the symmetry of the space when a crystallographic screw axis exists?
- 26) Why point groups are useful in crystallography?
- 27) Which is the role of the Laue group in crystallography?
- 28) You know that the 3d Bravais lattices are 14. Which is the general criterion fixing this number?
- 29) The following lattice parameters have been experimentally measured (within experimental errors): $a=21.30 \text{ \AA}$, $b=21.30 \text{ \AA}$, $c=45 \text{ \AA}$, $\alpha=\beta=\gamma=90^\circ$. Which is the crystal system?
- 30) You know that so far the crystals were assigned to one of the 7 crystal systems. But maybe you know that a new crystal system has been discovered, characterized by *a whichever, b whichever, c whichever, alpha whichever, beta whichever, gamma=90°*. Do you observe something against this statement?
- 31) Are you able to draw the equivalent positions for the space group $P2_1$ and Pc without checking the International Tables?
- 32) Are you able to derive the algebraic expressions of the symmetry equivalent positions for $P2_1$, Pc , $P3$ and $P4$?
- 33) How do you discover the space group symmetry from the diffraction pattern? Do you know the hierarchic sequence to follow for fixing the space group?
- 34) What an atomic scattering factor represents? What does a structure factor represents?
- 35) Does the amplitude of the structure factor depend on the atoms belonging to the asymmetric unit or on all the atoms in the unit cell?
- 36) When you start a crystallographic study, why do you want to know the phases of the observed reflections?
- 37) How do you estimate the electron density in the unit cell of your crystal?
- 38) Which type of information is provided by the diffraction amplitudes alone? Did you use this information in some of your crystallographic works?