Code: **QI853**

Name: **Introdução à Cristalografia**

Name in English: **Introduction to Crystallography**

Name in Spanish: **Introducción a la Cristalografía**

Subject type: **Weekly**

Approval Type: **Grade and frequency**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semestral / All periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**-**	**-**	**-**	**-**	**-**	**2**	**15**	**2**

Occurrence on curriculum:

Pre requirement: **QI145 or QI146**

Summary: Crystals and crystalline structures. Crystalline lattices and spatial symmetry. Crystalline systems. Diffraction in crystals: X-rays, neutrons and electrons. Introduction to the determination of crystalline structure. Examples of minerals, ionic and molecular compounds.

Program:

- Cell units and lattices and the diffraction experiment; reciprocal space and structural factors.
- Crystal symmetry; symmetry involving translation; crystalline systems and spatial groups.
- Experimental methods: processes and methods of crystallization; data collection for single crystals and polycrystalline samples. X-Rays, neutrons and electrons diffractions.
- Refinement of structures; Patterson and direct methods; minimum squares method. Disorder. Anomalous dispersion.
- Crystallographic databases.

Basic Bibliography

1) HAMMOND, C. **The basics of crystallography and diffraction.** 3rd ed. Oxford, N.Y.: Oxford University Press, 2009. 432p.

2) MASSA, W. **Crystal structure determination.** 2nd ed. Berlin: Springer, 2004. 210p.

3) CLEGG, W. **Crystal structure determination.** Oxford: Oxford University Press, 1998. 84p.

Supplementary Bibliography

1) CLEGG, W. (Ed.). **Crystal structure analysis: principles and practice.** 2nd ed. Oxford, N.Y.: Oxford University Press, 2009. 387p

2) GLUSKER, J. P. **Crystal structure analysis for chemists and biologists.** New York, N.Y.: VCH, 1994. 854p.

3) PECHARSKY, V. K. **Fundamentals of powder diffraction and structural characterization of materials.** 2nd ed. New York: Springer, 2009. 741p.

4) LADD, M. F. C. **Structure determination by X-ray crystallography.** 4th ed. New York, NY: Kluwer/Plenum, 2003. 819p.

5) RISSANEN, K. **Advanced X-Ray Crystallography.** Berlin, Heidelberg: Springer Berlin Heidelberg, 2012. (Topics in Current Chemistry; 315). E-book.