Please submit your answers electronically to email pavel.plevka@ceitec.muni.cz. Submit your answers as Microsoft word (.doc or .docx) or Portable Document Format (.pdf) documents. Make sure that you label your answers with question numbers. Some of the questions may require a drawing as part of the answer. In these cases, please use your mobile phone to take picture of your drawing and insert it into the document.
Deadline for sending the results is 5.2. 17:00.

Section A – Short essays. Answer as concisely as possible. Write equations or use drawings where appropriate. [10 points each].
(1) What is a unit cell?
(2) Why do crystals diffract X rays into "spots"?
(3) Why are X rays used for protein structure determination?
(4) Why do we need to scale diffraction data? How are diffraction data sets scaled? Write the equation for the scaling R factor.
(5) Draw and explain Argand diagram.
(6) How is the "free R-factor" calculated? Why do we use it?
(7) How is Fourier shell correlation (FSC) calculated?
(8) What is the wavelength of electrons used in electron microscopy (accelerating voltage 200-300kV). How can the wavelength be calculated?
(9) What is underfocus? – Use a drawing for the explanation.
(10) What is contrast, what are sources of contrast in EM?
(11) Explain what are centric reflections. Give examples of two spacegroups that contain centric reflections.

Section B – "Long" exercises. Please answer as concisely as possible. Write equations where appropriate. [20 points each]
(12) Demonstrate the systematic absences for space group with 2(1) screw axis along b. Symmetry operators are: (x; y; z) and(-x; y+1/2; -z)
(13) Write an equation representing non-periodic object with Fourier transform – explain the differences to the periodic situation applied in X-ray crystallography.
(14) A cubic crystal of iridium (Ir) is analyzed by X-ray diffraction through exposure to molybdenum Kα radiation, for which $\lambda_{K\alpha}$ = 0.721Å. Calculate the angle of reflection, θ, of the Bragg plane [1; 2; 0]. The unit cell length a = 10 Å.
If you wanted to increase the angle at which the reflection is observed, would you use X-rays with shorter or longer wavelength? Explain the reasoning behind your choice.

Section C – Equations. Write the equations. Define all the variables. [10 points each]
(15) Equation to calculate standard electron density map.
(16) Standard linear correlation coefficient between calculated and observed structure factor amplitudes.
(17) Crystallographic R-factor indicating correctness of a structure.
(18) Equation to calculate $2F_{Obs} - F_{Calc}$ map. What is this type of map good for?
(19) The inverse Fourier transform to calculate structure factors from electron density distribution.