Section A – Short essays. Answer as concisely as possible. Write equations or use drawings where appropriate. [10 points each].

(1) Draw a 2D lattice with a=b; α=90°. Draw and label the following lattice planes in the lattice: [2;1]; [3;2]; [-1;2]

(2) Explain why do crystals diffract X rays into "spots"?

(3) What is non-isomorphism? Why can't we combine X-ray data from non-isomorphous crystals, even if they contain the exact same molecules?

(4) Why do we need to scale diffraction data? How are diffraction data sets scaled? Write the equation for the scaling R factor.

(5) What is the resolution of the following reflections: [7;0;0], [0;10;0], [0;0;154], from a unit cell with parameters: a=456 Å, b=213 Å, c=254 Å, α=β=γ=90°. Does the resolution of the reflections depend on the wavelength used for the diffraction? If yes, what happens if the wavelength is decreased to 1/2? Explain all your answers.

(6) How is the "free R-factor" calculated? Why do we use it?

(7) How is Fourier shell correlation (FSC) calculated?

(8) Why do we use electrons in electron microscopes?

(9) What is Rayleigh criterion?

(10) What is underfocus? – Use a drawing for the explanation. How does it contribute to increased contrast?

(11) What are preferential orientations in EM? Do they constitute a problem for obtaining 3D reconstruction?

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) Explain amplitude and phase contrast. Use drawings. Explain how do the different types of contrast contribute to image contrast.

(14) Write an equation representing non-periodic object with Fourier transform – explain the differences to the periodic situation applied in X-ray crystallography.

(15) 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; 1; 0]. The unit cell length a = 3.84 Å.

If you wanted to increase the angle at which the reflection described in question (1) 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]

(16) Equation to calculate standard electron density map.

(17) R factor for comparing the intensity of symmetry-related reflections.

(18) Crystallographic R-factor indicating correctness of a structure.

(19) Equation to calculate $2F_{Obs} - F_{Calc}$ map.

(20) The inverse Fourier transform to calculate structure factors from electron density distribution.