

1. Please describe the basic principles of Nuclear Magnetic Resonance and Electron Spin Resonance; please explicitly provide two similarities and two differences between these methods.
2. Please describe the meaning of correlation between two quantities and explain how to evaluate the correlation level.
3. Please explain the concept of linear and non-linear regression and provide two examples of processes that can be modelled in that way (one linear and one non-linear). Please provide the mathematical formulations, explaining the meaning of the symbols used.
4. Knowing that in Electron Spin Resonance experiments one detects a derivative of the absorption signal, please explain the meaning of the first and the second integral of the signal. Is the statement that to determine the amount of free radicals in a sample one has to perform a double integration of the output of the experiment, true? Please explain.
5. Please provide examples of software development challenges associated with molecular modelling, using Gaussian as an example.
6. Please answer YES, NO to the statements below and explain your answer in 2 sentences for each point
 - a) The change in the sample magnetisation is related to absorption or emission of energy
 - b) Energy can be expressed in frequency units
 - c) Different parts of the electromagnetic spectrum correspond to electromagnetic waves of different energies
 - d) The energy of an electromagnetic wave of a lower frequency is higher
7. Please explain what criteria can be used to determine initial parameters, A, B and C, of a model described by the expression:
8. Knowing that diffusion processes become faster with increasing temperature, please decide whether the model:

$$y(x) = A * \exp\left(-\frac{x}{B}\right) + C$$

$$D(T) = A * \exp\left(\frac{E}{T}\right)$$

Where D denotes the diffusion coefficient, A - an amplitude and $E > 0$ is possible. T stands for temperature. Please explain the answer.

Advice: D for water at 20°C is about $2 \cdot 10^{-9} \text{ m}^2/\text{s}$, for 10°C this value is smaller.