Concorso pubblico anno accademico 2020/2021 per l'accesso al

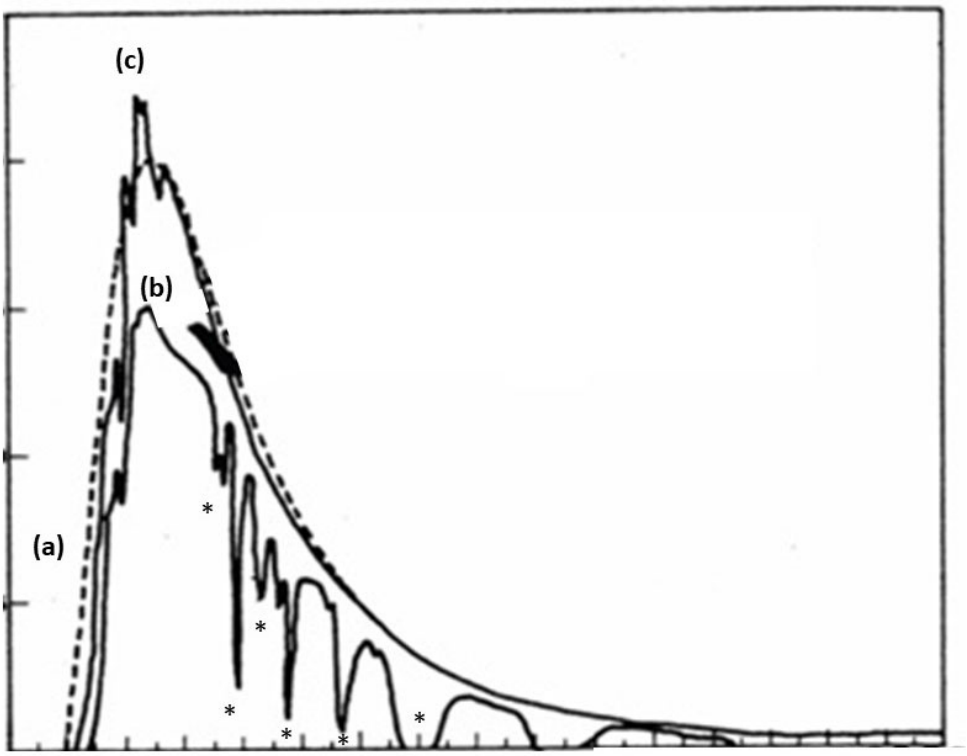
Corso di dottorato in "Scienze Chimiche e dei Materiali"

procedura concorsuale ordinaria

(bandito con decreto rettorale n.51936 del 10 giugno 2020 e successive modifiche e integrazioni)

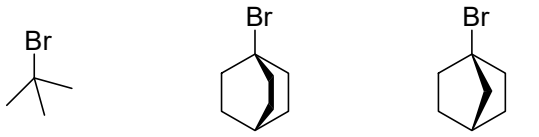
Questions/Problems:

1. Describe the parameters and operating choices for the optimization of an industrial chemical process.
2. This is a graph showing the spectrum of solar radiation as observed from the Earth. Indicate the appropriate labels of the x- and y- axes. Answer to the questions below:
   - Among these curves, which ones are theoretical and which ones are experimental ones? Explain the meaning of each curve and the main differences among the three curves.
   - Curve (b) presents several peaks, indicated with several asterisks. What is the origin of these peaks and their meaning from the chemical point of view?



3. Explain why a square planar or a tetrahedral geometry are sometimes preferred to an octahedral geometry in coordination chemistry. Discuss significant examples.
4. The use of high-resolution accurate mass spectrometry is spreading in research laboratories, but it's not all pros. Describe what are the disadvantages and outline the strategies to deal with them.

5. Explain the technical improvements and significant changes from the first IR spectrophotometers to the actual FT-IR spectrophotometers. Drawn them schematically and discuss the main optical elements of an IR spectrophotometer *versus* a FT-IR spectrophotometer.
6. Which are the general pre-conditions for the estimation of regression parameters (intercept and slope) by means of the ordinary least square, OLS?
7. Trends in the back-bonding ability of the metal, in transition metal coordination complexes. Discuss effects due to the nature of the metal, its oxidation state and the nature of ancillary ligands. From your answer, please suggest how you could design a transition metal coordination complex able to maximize back-bonding.
8. Nucleophilic substitution at a saturated carbon atom. Discuss the reaction mechanisms and the kinetic aspects. How could you rationalize the reaction rates determined for the solvolysis in aq. EtOH at 25 °C of the following bromo derivatives?



$k_{oss:}$ 1 ca. 10^{-6} ca. 10^{-14}

9. Describe the reasons and factors of deactivation of industrial catalysts.
10. Pericyclic reactions: definition and mechanistic aspects. Describe the products of the following Diels-Alder reaction and discuss the different kinds of selectivity that can operate: