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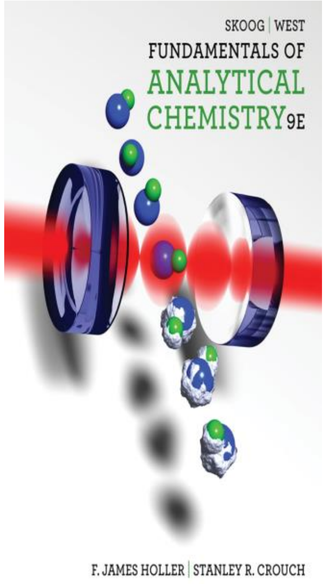
1.



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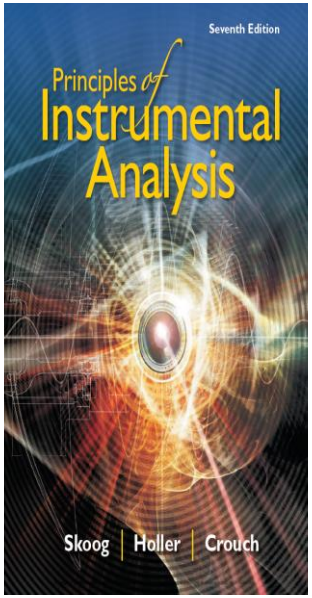

3.

ATAKOL's lecture notes

1. Skoog, D.A., West, D.M., Holler, J.F., Crouch, S.R. 2013. Fundamentals of Analytical Chemistry (9E). Cengage Learning, Belmont, USA.
2. Skoog, D.A., Holler, J.F., Crouch, S.R. 2016. Principles of Instrumental Analysis (7E). Cengage Learning, Boston, USA.
3. Prof. Dr. Orhan ATAKOL's lecture notes.

^{13}CNMR Method

- It is the most widely used NMR technique after ^{1}HNMR. However, since the signals obtained in the ^{13}CNMR method were too weak to be compared with the ^{1}HNMR method, their development occurred after 1980.

- Practically ^{13}CNMR spectra are spectra that help determine how many different carbon atoms are in the molecule, in other words, the carbon skeleton of the molecule. In this method, as in the ^{1}HNMR method, it is possible to determine the functional groups such as aromatic carbons, carbonyl, electronegative atom-bound carbons, etc.

- In the ^{13}CNMR Method, there is no spin spin interaction between the carbon atoms because the relative abundance of the ^{13}C isotope is 1.11%, and the probability of two ^{13}C isotopes coexisting is 1/10000, incidentally, the power of the devices cannot distinguish this split even if two NMR active nuclei are juxtaposed.

- In the ^{1}HNMR Method, the analyte is absolutely placed in the probe of the device in solution and while the spectrum is recorded, it is possible to record the spectrum of solid crystalline substances in the ^{13}CNMR technique.

- One of the best aspects of the ^{13}CNMR Method is that the standard is TMS again and the scale is quite wide. In ^{1}HNMR techniques, the δ scale ranges from 0-20 ppm, while in the ^{13}CNMR method there is a scale ranging from 0-220 ppm for many compounds, so it is possible to select all the different carbons in the spectra of substances whose molecular mass is not very large.

- According to the ^{1}HNMR method, it is the absence of a single side integration feature. In other words, the number and properties of different carbon atoms can be chosen, but no information about their quantitative ratios relative to each other can be obtained from this method because the location of the ^{13}C isotopes in the molecule is random. It also gives an idea of the amount of different carbon cores, but this is not as clear as in the ^{1}HNMR method. The signal of the large number of carbon atoms is relatively larger.

- In ^{13}C NMR Method, as in ^{1}HNMR, carbon atoms give different sinyal values according to the functional group they are in.

- There is no spin spin interaction between carbons in ^{13}C NMR spectroscopy, but one thing we know in all NMR technique is that all NMR active nuclei participate in spin spin interaction (NMR active nuclei cause spin spin cleavages depending on the number of nuclei of the nucleus). So these C atoms are connected to H atoms and these H atoms are NMR active nuclei and they are very close to C atoms. Therefore, hydrogen atoms cause spin spin interaction in ^{13}C NMR spectra.

* The hydrogens in the CH3 group are quartets, hydrogens in the -CH2- group include carbon to which they are attached triplet and hydrogens in the group -CH = turn the carbon to which they are attached to double.

This explanatory in the 1HNMR method, which helps in solving the spectrum, can help explain the spectrum in the 13CNMR method, as well as interfering with close signals. This spin spin splitting caused by hydrogen in close proximity signals can cause errors in determining the number of different carbon atoms in the carbon skeleton.

- For this reason, 13CNMR spectra are recorded in two ways,

1- Spin spin interaction created by hydrogens without removing (without decapling)

2- By eliminating the spin spin interaction created by hydrogen (by decoupling).

- Decapling is a technique that is applied from time to time in the 1HNMR method, but is always applied in the 13CNMR method. It is an application performed by not using the resonance nuclei to participate in the spin spin interaction.

- A second field during the recording of the spectrum is a technique based on the resonance of other nuclei that cause spin spin interaction with the scanning system. Since the radiofrequency absorbed by the nuclei that cause spin spin interaction is different, a second magnetic field scan and radiofrequency do not harm the spectrum that is desired to be recorded. There are several different methods of decoupling applications. These are:

  Broadband technique,

  Pulsed decapling and

  Remote resonance technique.