THE COMPUTERPROGRAM "HELP-IR" FOR HELPING THE INTERPRETATION OF IR-SPECTRA

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Summary

A brief description is presented about the "Help-IR" computerprogram. The program is written in FORTRAN of the Aspect 2000 minicomputer of the Bruker IFS 113v IR-spectrometer. It is hoped that the program will be able to support an effective help in interpreting of IR-spectra of the common organic compounds.

The purpose of the program

Two main directions can be observed in the development of the computer-aided IR-spectra interpretation: the "mathematical" search and the "chemical-spectroscopical" method. In the "mathematical" search the unknown IR-spectrum is compared with the elements of a representative IR-spectra library. In the "chemical-spectroscopical" method the practical-empirical rules are organized to a computer program. The "mathematical" method suffers despite of his advantages in a main disadvantage, namely it needs an IR-spectra library. Such a library is not freely available in any case. In contrary to it the "chemical-spectroscopical" method can freely use the great amount of informations about the IR-characteristics of the organic compounds. These informations are summarized usually in correlation charts and they can be found in the standard books of the IR-spectroscopy.

The "Help-IR" program can be considered to such a correlation chart written in the memory of a computer.

The structure of the program

The program is written in FORTRAN of the Aspect 2000 minicomputer built in the Bruker IFS 113v IR-spectrometer.

The input data are the following:

— the number of the peaks involved in the interpretation (max. 30),
— the positions of the peaks in wavenumber unit,
— the codes of intensity of the peaks (1 = strong, 0 = not strong, 2 = undetermined),

— the answers to the questions of the chemical filter: additional informations relating to the elemental content and the chemical structure of the sample (if these are known in some extent) (max. 62 questions).

The input of these data is executed in interactive way through the teletype between the user and the computer.

The MASTER block organizes all functions in the program, it selects the appropriate subroutines in the MODULES block depending on the answers of the chemical filter.

The MODULES block contains the correlation charts of the different groups of the common organic compounds. These data are taken from the well-known standard books of the IR-spectroscopy [1–5].

The names of the organic compounds incorporated into the program are listed in Table 1. The number in parentheses tells the number of spectroscopical rules relating to the particular group of compounds.

After the first selection by the chemical filter the program executes a second selection based on the input data. The program examines in the LLOP block the position- and intensity-data of the spectrum and determines what type of functional groups can be present in it. This decision is made by the inspection of the simultaneous presence of some preselected principal peaks characteristic to the particular functional group. If all of the principal peaks are found, the program prints out in the PRINT block the stored informations about the principal and the additional peaks characteristic to the functional group.

The output data are the following:

— the position of the selected peak in wavenumber unit,

— the names of the predicted functional groups assigned to the selected peak.

Table 1

The groups of organic compounds, which can be interpreted by the "Help-IR"

S-compounds	(43)	carboxylic acids	(13)
P-compounds	(21)	anhydrides	(10)
X-compounds	(25)	halides	(2)
amines	(35)	esters	(24)
amides	(47)	lactones	(6)
lactames	(8)	alcohols	(23)
amino acids	(28)	ethers	(34)
unsat. N-compounds	(25)	peroxides	(12)
pentavalent N—O	(32)	alkanes	(43)
trivalent N—O	(23)	alkenes	(55)
ketones	(34)	alkines	(5)
aldehydes	(11)	benzene ring	(46)

— the intensity of the peak of the predicted functional group,
— the names of the compounds, which may contain the predicted functional group,
— the spectroscopical type of the vibration,
— other helping remarks for the assigment of the peak.

It should be noted that the PRINT subroutine enables us to distinguish between five classes of intensity (1, weak, 2. weak-medium, 3. medium-strong or variable, 4. strong, 5. very strong).

Further development of the program

So far 194 IR-spectra have been successfully interpreted with the "Help-IR" program. It should be said that the program in its present state is far from the completeness. Further developments should be made in two directions. An improvement in the selectivity should be achieved taking into account additional spectroscopical characteristics (e.g. weak but characteristic peaks, linewidth, etc.) and the MODULES block should be completed by additional important organic compounds (e.g. heteroaromatic rings, etc.). These developments can be easily done because of the modular structure of the program.

References

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