

- Spectrometric data depend on the instrumentation as well as on the physical state of the compounds and the operating procedures. For instance, it is accepted in mass spectrometry that, with the present state of the art, it is not feasible to obtain spectra that are independent of the instrumentation (3). A data base containing spectra from different sources will therefore be more realistic, especially if the accredited laboratories use different types of instruments.
- As spectrometric data depend on the instrumentation one may have to consider to start all over again whenever analytical equipment is replaced.

The major disadvantage of creating an instrumental data base consisting of data obtained from different laboratories seems to be the fact that it will lead to non-uniformity. For certain types of spectrometry this will certainly be the case, but the question is whether that really matters. If a spectrum varies essentially when it is obtained with different instruments, this spectrum can never be the basis for a sound identification. Moreover, identification has to be considered as a subject for specialists which should be capable to interpret differences occurring eventually between the recorded spectra and the ones in the data base. They should also be aware of the fact that blind acceptance of reference data may lead to misinterpretation as was recently demonstrated (4).

Thus far, only Finland has systematically presented its collected spectrometric and chromatographic reference data. A series of Blue Books (5) was published prior to the start of the Verification Data Base (6) which will include all Finish recorded data. The Netherlands has also collected reference data of compounds of CW interest. These data were obtained mainly from compounds which were prepared in the PML-TNO laboratory in Rijswijk. This collection started some twenty years ago, first in the form of printed spectra. After the introduction of spectrometric data systems the collection was converted into a computerized data base. Data can be made available in several formats. Special parts of the compiled mass spectral data were occasionally published (7-10). Other nations have indicated that they possess useful data. For instance, D'Agostino and co-workers from the Canadian DRES laboratory in Suffield have published several papers containing gas chromatographic data (retention indices) as well as electron impact (EI) and chemical ionization (CI) mass spectra of CW agents and other compounds of CW interest (11-18).

If the states represented in the Technical Group on Instrumentation would agree with the Netherlands view to create an instrumental data base from existing data, an inquiry might be held in which the states indicate the kind of data they are willing to provide. The data base will then be constructed in more or less the same way as the reference data collection for mass spectra in the NIST/EPA/MSDC data base (19). The major concern of such a file of 40.000 mass spectra is the quality of the spectra it contains. It is almost impossible to check manually each spectrum in such a large compilation. Therefore each spectrum in this file was evaluated by calculating a set of quality factors using a computer programme (20,21). It is obvious that these quality factors can be calculated for the mass spectral data of compounds of CW interest. It should be investigated whether similar quality factors could be deduced for other spectrometric as well as the chromatographic techniques. The number of compounds in the instrumental data base for verification will be limited and possibly not exceed 500. A selected group of experts might form an editorial board and give their opinion on each entry.

### 3. Instrumental data to be collected

A survey of the instrumental data which should be incorporated in a data base is presented in a report of the Technical Group on Instrumentation (2). Although in principle each piece of information might have its value, some data are more important than others. The order of importance can be deduced from the criteria for confirmation of CW agents identification, which have been proposed by The Netherlands (22). The following order is proposed :