reference standards have to used. Accordingly no prerecorded parameters can be stored in a database.

Mass spectrometry (MS)

20. MS is the most widely used spectrometric technique in verification analysis. The spectra depend to some extent on the type of instrument and recording conditions. For the evaluation of the quality, it is essential to include details of the recording conditions and the purity of samples with the spectra. Quality indices have been introduced to aid the assessment (Terwillinger et al., Biomed. and Environ. Mass Spectrom. 14, 263-270 (1987)). There are no universally accepted recording conditions. However, international recommendations have been made, and laboratories which do not have extensive experience might be adviced to use conditions described in literature (e.g. Dillard et al. Org. Mass Spectrom., vol 16, pp. 48-49, 1981 or Blue Book, F.1, 1990).

21. In general, the most valuable information for mass spectrometrist is the positive electron ionization spectra recorded using 70 eV. Positive chemical ionization spectra recorded using isobutane, methane or ammonia as reactant gases were also considered useful. For those compounds for which negative ion spectra are more sensitive than positive ion spectra, these spectra should be included. The high resolution MS and MS/MS data, while not considered essential, provide additional information for the analysts, and, when available, should be included in the data base.

Infrared spectrometry (IR)

22. The Coblentz Society has published specifications for the recording of infrared spectra. Specifications are described for gas-phase spectra and for condensed-phase spectra (Applied Spectroscopy, vol. 44, pp. 211-215 (1990) and Analytical Chemistry, vol. 47, pp. 945A-952A (1975), respectively). It was noted that the new deposition technique produces spectra from sub-nanogram quantities of chemicals and allows spectral comparison with those in the condensed-phase libraries. Detailed recording conditions are included in the specifications and should follow the spectra submitted for the data base. Published quality criteria are available to aid selection of spectra.

23. There are numerous spectra of relevant chemicals recorded well before any specifications were established. The Group recommends that these spectra be included in the data base when new data have not been recorded.

24. In the central data base the spectra should be stored as interferograms, when possible, to allow later reprocessing of spectra.

Nuclear Magnetic Resonance Spectrometry (NMR)

25. The NMR database should include ^{1}H, ^{13}C, ^{31}P, and ^{19}F spectra. The spectra should be recorded in different deuterated solvents.