

As for the analytical reference data itself, of primary importance to the analytical community, is that both spectrometric and chromatographic data for all compounds in the database must be included. This leads to the question of how will these data be obtained. We generally support the concept that the chromatograph and spectra should be solicited from the laboratories which have been active in the field and which have experience in the identification of chemical agents. Other data especially spectra of precursors and degradation products, may be available in commercial databases and the chemical literature. Other sources of standard spectra of organic compounds in the U.S. are the National Institute of Standards and Technology, (formerly the National Bureau of Standards), the Environmental Protection Agency and the National Institutes of Health. Similar sources are available in other countries. There will, in all probability, be multiple sets of data available for each material. Rather than including all data in the database, quality tests must be used to evaluate the available data and select only one set for inclusion in the database. Such tests have been developed by the U.S. Environmental Protection Agency and others. These techniques are available to ensure that only the highest quality data is included.

The selection of the types of spectra to be included in the database is a critical issue that depends to some extent on whether the analyses are to be performed on-site during an inspection or at a fixed laboratory off-site. The types of instruments which can be used on-site or in a mobile laboratory will limit the spectra to be included in the database. For on-site use, we propose that gas chromatography (GC) retention times, electron impact (EI) mass spectra would certainly be included. Infrared (IR) spectra would also be desirable. The instrument operational conditions under which the data were obtained would be specified in agreement with the prescribed analytical standard operating procedure; i.e., GC temperature/flow rate conditions, GC column type, etc., mass spectrometer ionizing voltage, etc., additional data for use in off-site laboratories, where more sophisticated instruments will be available should also be included for referee or reference laboratory use. These would include nuclear magnetic resonance (NMR) spectra and possible others which would be needed for structure elucidation if that is desired.

A separate database section should be developed comprising the reference analytical procedures, i.e., standard operating procedures for the instruments selected to be used in the verification process. A necessary part of this procedural database would be standard sampling procedures for all types of samples that may be encountered during an inspection, i.e., process samples, environmental samples, etc., and standard packaging,