

ABSTRACT OF THE DISCLOSURE

A method of operating a spectrometer to determine property and/or composition data of a sample comprises an on-line spectral measurement of the sample using a computer controlled spectrometer, statistical analysis of the sample data based upon a statistical model using sample calibration data, and automatically identifying a sample if necessary based upon statistical and expert system (rule-based) criteria. Sample collection based upon statistical criteria consists of performing a statistical or rule-based check against the model to identify measurement data which are indicative of chemical species not in the samples already stored in the model. Samples identified either by a statistical criteria or using an expert system (rule-based decisions) are used preferably to isolate the liquid sample using a computer controlled automatic sampling system. The samples can be saved for subsequent laboratory analysis in removable sample containers. The results of the laboratory analysis together with the on-line spectroscopic measurements are preferably used to update the model being used for the analysis.