

Gas Analysis | EGAsoft
Technical Information TI-20006.1

EGAsoft

Data Acquisition Software for TA-MS

TA-MS

Hyphenated techniques using evolved gas analysers such as TGA-MS or DSC-MS are becoming increasingly important in thermal analysis applications. For evolved gas analysis, Hiden produce the HPR-20 EGA mass spectrometer system with optimized inlets for any TGA/DSC system. Coupled to the HPR-20 EGA is Hiden EGAsoft, a complete, application specific, software package for EGA data acquisition and analysis. Features include:

- 3D bar scan view for easy determination of trends in bar data.
- Simple automatic export in formats

- specific for import to any TGA/DSC manufacturer.
- Automatic spectral deconvolution in MID mode.
- Peak integration and data analysis routines.
- Auto-sequencing of MS data acquisition files e.g. for use with auto samplers.
- Auto start/stop and temperature inputs where output signals are available.
- Mass spectrometer ionisation energy control for soft ionisation of complex mixtures.

Features

EGAsoft has many features designed to make MS data acquisition easy in TA-MS experiments. The main features are described below.

3D Bar Scan

Figure 1 shows the 3D bar graphing feature. This data display allows easy identification of trends in the MS data. This is especially important as in many TA-MS experiments the decomposition products are not always known before the experiment begins.

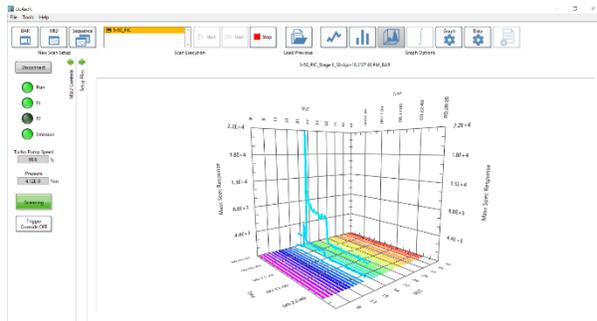


Figure 1: 3D Bar Mode

The 3D view is fully rotatable and specific areas of interest can be selected during the experimental run to identify peaks of interest.

Trends can then be displayed in MID (multiple ion detection) mode, see Figure 2. A 2D bar mode, Figure 3, shows the current Bar scan or can be used to analyse the bar scan from specific points of the MID scan.



Figure 2: MID Mode

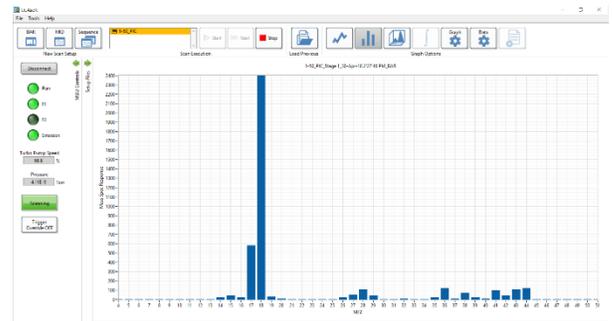


Figure 3: 2D Bar Mode

For analysis of known desorption species a MID scan can be configured to only analyse these species improving signal acquisition rates and detection capabilities.



Figure 4: MID setup

Auto-sequencing

TGA systems are often fitted with autosamplers. If different samples are being run then it is often desirable to have an optimized MS setup for each sample. The EGAsoft auto-sequencing feature enables the user to configure any number of different sequences of MS scans, Bar or MID, and save them as templates to be run repeatedly. Figure 5 shows the auto-sequencer screen from EGAsoft.

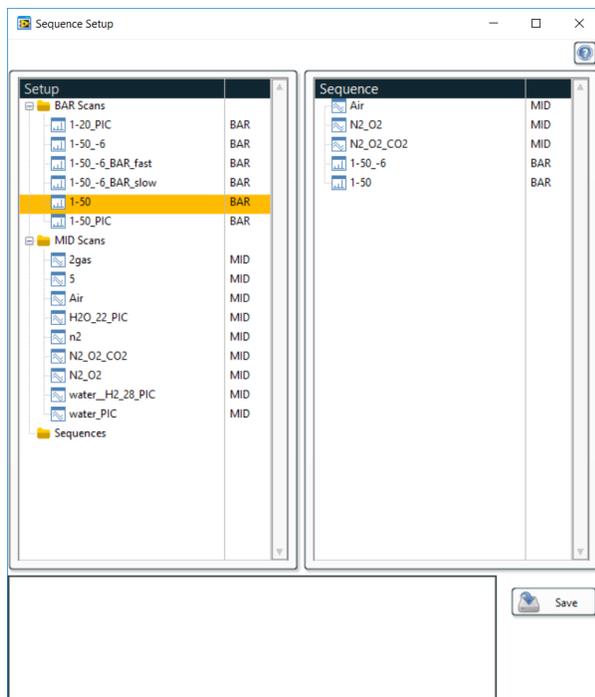


Figure 5: EGAsoft Sequencer

Spectral Deconvolution

When detecting specific gases with the MS, users must be aware of any spectral overlaps that may occur from the fragmentation process during ionisation. If these are not taken into account then species can be wrongly identified. When using EGAsoft in MID mode the software will automatically identify any spectral overlaps in the chosen gases and subtract these to give only the MS intensity of the

desired species. An example of this is shown in Figure 6. This shows the analysis of CO₂, O₂ and CO. CO₂ has a mass contribution at m/z 28. This causes an overlap with the CO at m/z 28. Here the software will recognize this and remove the CO₂ contribution at m/z 28.



Figure 6 - MID Setup

The MID mode setup also allows the easy configuration of different ionization energies for different species. This can help when detecting species that have multiple overlapping peaks. Soft ionisation allows the preferential ionisation of species and can minimize the fragmentation overlaps from complex molecules.

Peak Integration

EGAsoft features an easy to use peak integration and deconvolution package. Desorption peaks are automatically integrated over the selected range with baseline correction and subtraction as shown in Figure 7.



Figure 7: Baseline Subtraction

If the peak has several overlapping features then they can be deconvoluted using multiple Gaussian curves to determine quantities of gas desorbing or decomposing from different sites or processes. Peak integration and deconvolution are shown in Figure 8.

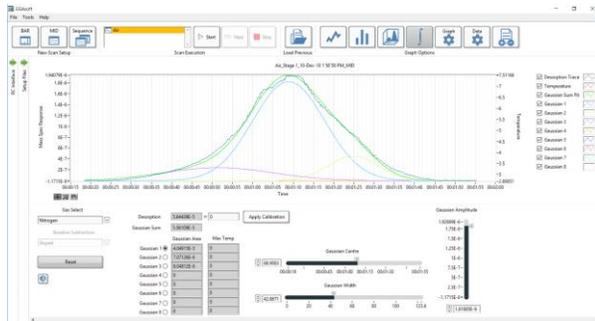


Figure 8: Peak Deconvolution & Integration

Data can be exported in report format for a permanent record of the peak analysis. An example of the report is shown in Figure 9.

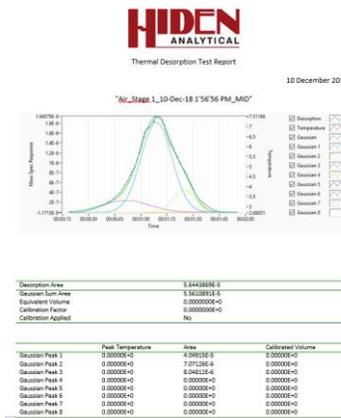


Figure 9: EGAssoft Experimental Report

Additional Features

In addition EGAssoft also includes features such as:

- Data smoothing and data point removal functions.
- One-click export in file formats for direct import in to TGA manufacturer software packages.
- Export selectable spectra to NIST mass spectral database for use of its comprehensive search features.
- Data display as temperature vs. MS response where external temperature signals are available.

These features combine to give the most complete MS data acquisition and analysis package available for use in thermal analysis applications.

Applications

EGAssoft can be used for all types of thermal analysis experiments including:

- TGA-MS
- UHV TPD/TDS experiments
- Atmospheric pressure TDS/TPD
- Catalysis temperature programmed studies (TPD/R/O)