Interior Air Analysis of a New Office Cabinet

LECO Corporation; Saint Joseph, Michigan USA

Key Words: GC-TOFMS, Environmental, Deconvolution

1. Introduction

The interior air of a new office cabinet was to be analyzed. The cabinet showed a clearly perceptible solvent smell, which needed to be investigated regarding its contents.

2. Experimental Conditions

Using a common gas-tight Hamilton syringe, 50 µL of air was taken from the cabinet interior and introduced to the GC-TOFMS system by means of split injection. The individual measurement parameters were as follows.

GC Parameters
Column:
J&W® DB-5 MS; 20 m x 0.18 mm x 0.18 µm
Injector Temperature: 180°C
Split Rate: 10:1
Heating Program:
30°C initial temperature, with 60°/minute to 240°C, hold for 0.3 minute
Flow Rate:
0.8 mL/minute Helium constant flow

MS-Parameters
Mass Range: 35 to 400 amu
Scan Rate: 30 spectra/second
Ion Source Temperature: 170°C
Total Run Time: 228 seconds

3. Results

In Figure 1 the Total Ion Chromatogram (TIC) of the measurement is shown. Only the argon signal is visible as a clear peak as the remaining main components present in air (nitrogen and oxygen) are faded out of the scanned mass range.

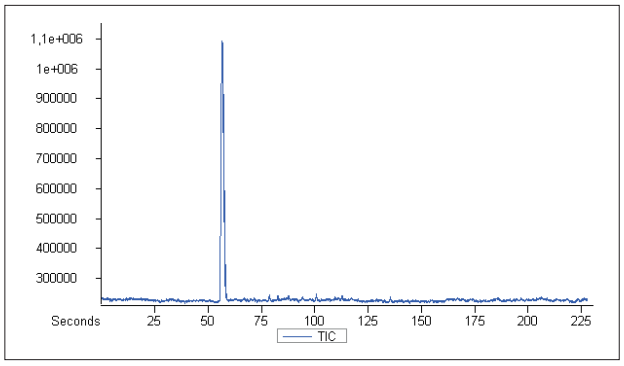

Figure 1. TIC of the cabinet air sample.

Using the Pegasus data processing software, the chromatogram was automatically searched for peaks. Since all mass traces are being considered, it is possible to find signals even below the baseline and identify those signals according to the deconvoluted mass spectra.

Although the sample initially appeared uncontaminated, a large number of different substances were found by the Automatic Peak Find algorithm. Those contaminants were mainly hydrocarbons. The identified substances are shown in Figure 2 as background corrected TIC (AIC).

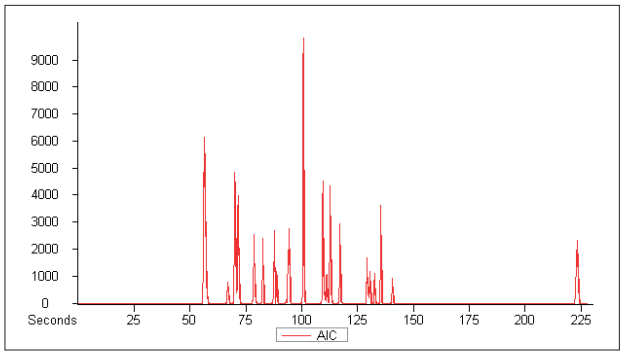

Figure 2. Analytical Ion Chromatogram (AIC) of the cabinet sample.

In total, 21 substances were identified according to their mass spectra. One of the main components, at approximately 100 seconds RT, was identified as acetic acid butylester. The deconvoluted spectrum and the corresponding library spectrum are shown in Figure 3.

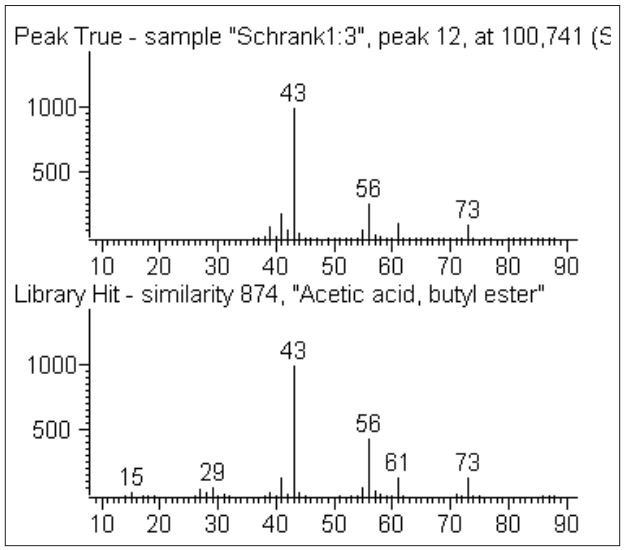

Figure 3. Measured spectrum and the corresponding library spectrum of acetic acid butylester.

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Other main components were identified as Cyclohexane, Heptane, Toluene, Xylene, and Trimethyl-benzene. The peak list is shown in Table 1.

Table 1. Peak list of air measurement.

Peak	Name	Similarity	R.T.
1	Argon	919	56.541
2	Silanol, trimethyl-	401	66.974
3	2-Butanone	814	70.108
4	Ethanethioic acid	458	71.574
5	Cyclohexane	887	78.674
6	Heptane	506	82.674
7	Cyclohexane, methyl-	806	87.808
8	Pentanal, 2,4-dimethyl-	661	88.808
9	Acetic acid, 2-methylpropyl ester	973	93.908
10	Toluene	728	94.474
11	Acetic acid, butyl ester	874	100.74
12	1-Methoxy-2-propyl acetate	792	109.47
13	Ethylbenzene	902	111.17
14	Benzene, 1,2-dimethyl-	920	112.74
15	Benzene, 1,2-dimethyl-	845	117.14
16	Benzene, 1-ethyl-4-methyl-	564	129.21
17	2,4-Nonadiyne	777	129.87
18	Benzene, 1,2,4-trimethyl-	558	130.61
19	Benzene, 1-ethyl-2-methyl-	588	132.61
20	Benzene, 1,2,3-trimethyl-	723	135.41
21	2,4-Nonadiyne	545	140.57
22	Dibutyl phthalate	635	223.24

With some of the substances in the chromatogram coeluting, the Pegasus deconvolution software mathematically separates the spectra of the overlapping compounds and provides undisturbed spectra as shown in Figure 4.

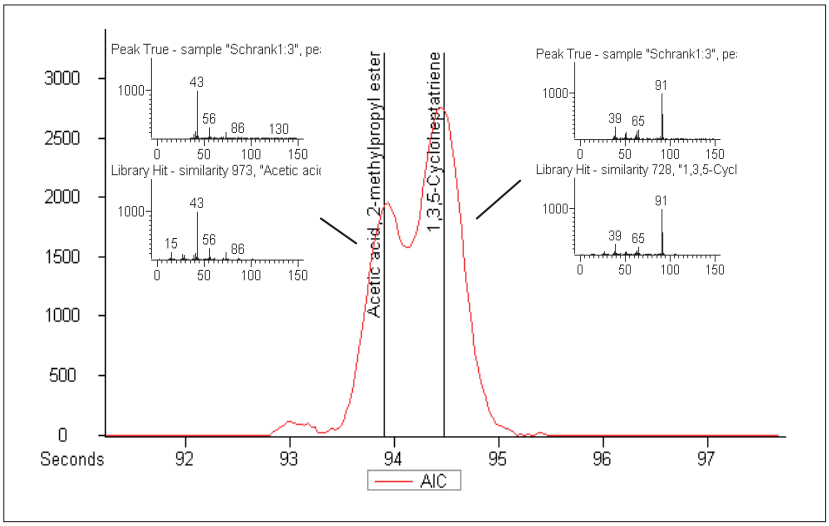

Figure 4. Coeluting substances and their deconvoluted spectra.

4. Conclusion and Outlook

The described application proves that the Pegasus is well suited for both gas and air analysis. Gas chromatographic analyses can be performed quickly, while providing excellent sensitivity. The data processing software not only allows the detection of unknown substances from the total ion current (even when the components are buried well below the baseline), but can additionally separate overlapping spectra and conduct a library identification.

The system's maximum scan rate of 500 full mass spectra per second allows for further acceleration of such a method. In addition, quantitative analysis can also be conducted, provided corresponding calibration standards are available.

LECO Corporation • 3000 Lakeview Avenue • St. Joseph, MI 49085 • Phone: 800-292-6141 • Fax: 269-982-8977
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