MARKES international

Application

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Application Note 033

Analysis of the interior atmosphere of a passenger car by TD–GC–MS

Summary

This Application Note describes the TD–GC–MS analysis of potentially harmful volatile organic compounds in the air of two new cars.

Introduction

Many of the fittings used in car interiors are known to emit volatile organic compounds (VOCs), which may cause odour problems as well as being hazardous to health. The range of compounds used in interior fittings can include alkanes, aromatic hydrocarbons, nitrogen compounds, terpenes and sulfur compounds. High temperatures and humidities can also increase the concentrations of some pollutants.

There has long been concern over exposure to such compounds, and this has been reflected in the development of methods to determine levels of VOCs and SVOCs in car interiors. In this Application Note we show how TD–GC–MS can be applied to the problem of analysing compounds spanning a wide range of volatilities and concentrations.

Experimental

Calibration:
Calibration used a 2 µL injection of a benzene, toluene and *m*-xylene standard in methanol (Figure 1). The solution was introduced onto a Tenax TA tube in a stream of carrier gas using the Calibration Standard Loading Rig (CSLR™, Markes International). Using the response for toluene as a convenient average, a peak area of 1.1 × 10^7 counts equates to approximately 20 ppb in the vehicle atmosphere.

Vehicles:
The cars used in these experiments were new standard 'compact' models with the windows and doors kept closed. As material emissions increase with rising temperature, the cars were sampled at ambient temperature and 40°C (to simulate the temperature reached inside a parked car in full sun).

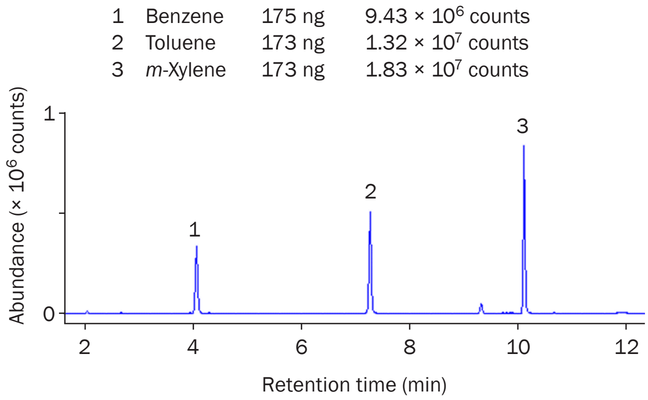

Figure 1: Analysis of a standard solution of benzene, toluene and *m*-xylene.

Sampling:
In all cases, 2 L of air from inside the cars was pumped at a rate of 50 mL/min onto sorbent tubes packed with Tenax® TA and Carbograph™ 1TD.

TD:

Instrument:	UNITY™ (Markes International)
Prepurge time:	1 min
Tube desorb:	275°C (6 min), split on
Trap low:	30°C
Trap desorb:	300°C (3 min), split on
Trap:	Tenax TA–Carbopack™ B
Flow path:	200°C
Carrier gas pressure:	10 psi
Desorb flow:	20 mL/min
Split flow:	30 mL/min
Split ratio:	75:1

GC:

Instrument:	Agilent 6890 GC
Column:	30 m × 0.32 mm × 1.0 µm DB1 equivalent (non-polar) phase
Oven ramp:	40°C (5 min), 10°C/min to 200°C (1 min)
Column flow:	~1 mL/min

MS:

instrument:	Agilent 5973 MSD
Source temp.:	230°C
Quadrupole temp.:	150°C
MSD transfer line:	280°C
Mass scan range:	m/z 45–350

Results and discussion

Figure 2 and Table 1 present results for: Model X with standard upholstery at (A) 20°C and (B) 40°C; (C) Model X with leather upholstery at 20°C; (D) Model Y at 20°C.

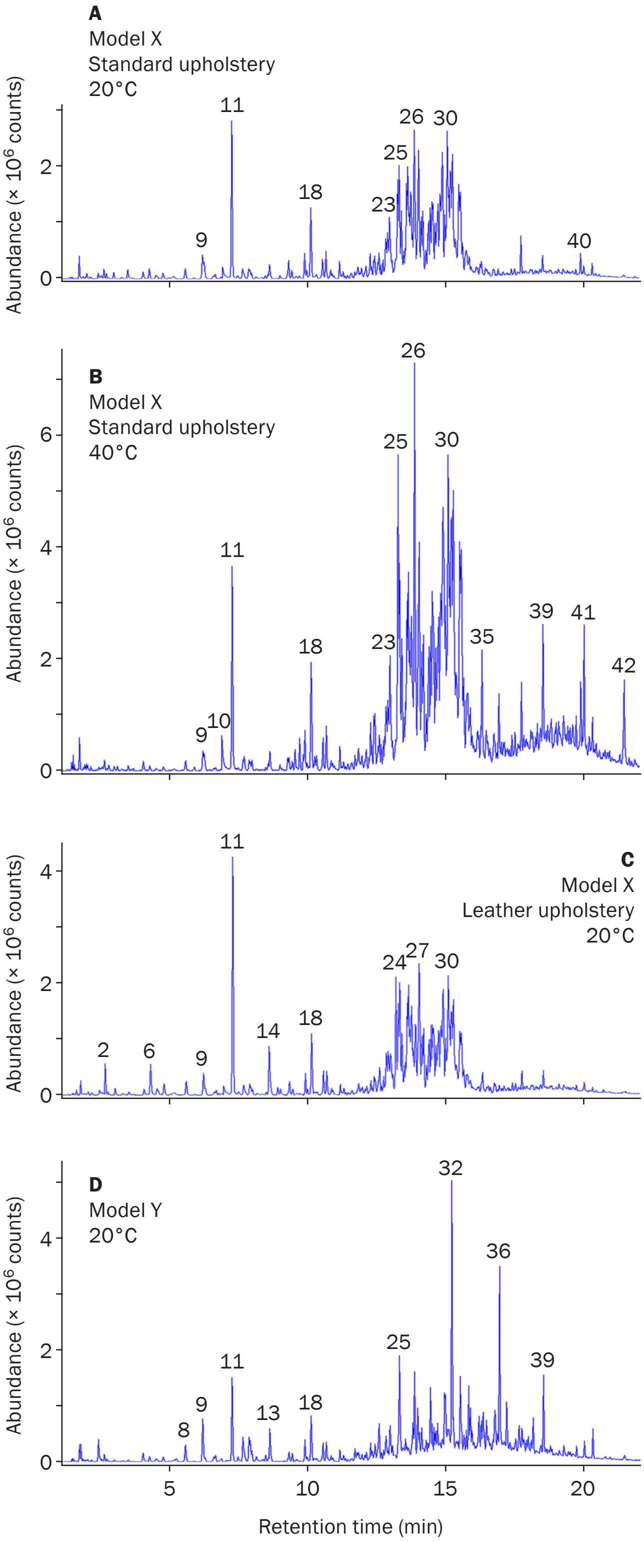

Figure 2: TD–GC–MS analyses of air from vehicle cabins.

No.	Compound name	Peak area (× 10^6 counts)			
		A	B	C	D
1	Trimethylsilanol	–	–	–	9.1
2	Methyl ethyl ketone	3.3	–	10.9	–
3	Ethyl acetate	–	–	2.8	–
4	n-Hexane	3.0	–	–	–
5	Benzene	3.3	–	2.9	4.0
6	Cyclohexane	4.6	–	17.9	–
7	Isoheptane	–	–	6.5	–
8	n-Heptane	5.7	–	7.6	9.2
9	Methylcyclohexane	12.0	9.6	15.4	19.3
10	*N*,*N*-Dimethylformamide	7.3	19.2	6.0	–
11	Toluene	74.8	93.4	112.4	38.6
12	Isooctane	7.0	–	7.0	15.8
13	n-Octane	7.2	–	–	16.1
14	Tetrachloroethene	–	–	27.4	–
15	Methoxybutanol	–	–	2.8	–
16	4-Hydroxy-4-methylpentan-2-one	–	–	2.4	–
17	Ethylbenzene	9.9	18.1	8.4	8.1
18	*m*-/*p*-Xylene	36.5	57.2	30.0	22.1
19	Styrene	9.5	14.5	10.7	8.4
20	*o*-Xylene	13.3	19.2	11.2	9.7
21	n-Nonane	7.4	8.6	–	–
22	Ethyltoluene	6.4	–	–	–
23	Trimethylbenzene	26.0	46.0	–	15.4
24	Propylene glycol diacetate	–	–	45.2	–
25	n-Decane	37.7	124.3	44.1	42.8
26	Dimethylbenzylamine	70.0	194.3	–	36.5
27	$C_{11/12}$ isomer	65.0	124.1	72.3	–
28	*trans*-Decalin	–	–	–	21.2
29	$C_{11/12}$ isomer	69.7	110.1	64.0	–
30	C_{12} isomer	50.4	94.9	37.1	–
31	C_{13} isomer	44.3	–	–	–
32	n-Undecane	–	–	–	98.0
33	Methyldecalin isomer	–	–	–	31.0
34	Methyldecalin isomer	–	–	–	24.1
35	2-(2-Butoxyethoxy)ethanol	5.5	56.9	9.4	–
36	n-Dodecane	–	28.0	–	66.9
37	C_{13} isomer	–	–	–	18.6
38	C_{14} isomer	–	–	–	13.9
39	n-Tridecane	6.4	48.5	6.3	27.5
40	Cubebene/Copaene	7.8	28.5	–	–
41	n-Tetradecane	–	44.1	3.3	5.7
42	Butylated hydroxy toluene	–	42.0	–	2.8
Total peak area		2038	5349	1893	1480
Total organics in 2 L air (µg)		26.6	9.7	24.7	19.3
TVOC (as ppm toluene equiv.)		**3.7**	**9.7**	**3.4**	**2.7**

Table 1: TD–GC–MS analyses of air from vehicle cabins.

Considering Model X, there is an approximate three-fold increase in TVOC (in toluene equivalents) on raising the internal temperature from ambient (Figure 1A) to 40°C (Figure 1B), with a shift in emphasis from the more volatile to the less volatile components.

The change from standard to leather upholstery in (Figure 1C) appears to be responsible for the appearance of several new analytes – the most significant being tetrachloroethene (#14, a dry-cleaning agent) and propylene glycol diacetate (#24, a high-boiling solvent/finishing agent).

The overall VOC profile of the air taken from Model Y (Figure 1D) is quite different from Model A, with a decrease in TVOC, but the appearance of several lower-volatility hydrocarbons.

Conclusions

Pumped sampling in conjunction with TD–GC–MS has been shown to be a useful method for the analysis of VOCs and SVOCs in car cabin air. A wide range of compounds can be screened, and comparision made between different models, allowing information to be obtained about the source of individual components.

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