



Application Note
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Monitoring Isocyanates Using a Bruker Ion Mobility Spectrometer

Both stationary and handheld ion mobility spectrometers (IMS) were used to monitor ambient air to sensitizing concentrations of toluene diisocyanate (TDI both 2,4 & 2,6 isomers) as well as Hexamethylene diisocyanate (HDI). The Bruker RAID (Rapid Alarm and Identification Device) series of instruments achieved detection limits down to 1 ppb (0.007 mg m^{-3}) within a few seconds, which is below the current workplace exposure limits.

Introduction

Isocyanates are increasingly being used for manufacturing polyurethane foam, elastomers, adhesives, paints, coatings, insecticides, and many other products. Despite the wide range of useful applications, they are regarded as dermal and inhalation sensitizers causing occupational asthma, lung damage and in severe cases fatal reactions. For this reason, the protection of workers from excessive exposure to TDI/HDI is an indispensable prerequisite. Ion mobility spectrometry is a fast and sensitive method of detection for a variety of harmful chemical vapors ranging from chemical warfare agents to toxic industrial chemicals. Bruker offers this fast, versatile and flexible responding detection technology in a variety of detector platforms, ranging from battery operated, lightweight, handheld point detectors (RAID-M 100) to fixed site continuous monitors (TIMON). This application note describes the usage of IMS devices for workplace monitoring to TDI/HDI exposure.

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Keywords	Instrumentation & Software
Toluene diisocyanate (TDI)	TIMON
Hexamethylene diisocyanate (HDI)	RAID-M 100
Occupational exposure limits	XIMS PLUS 1.0
Ion mobility spectrometry	

Experimental

Diverse Bruker IMS devices (TIMON, RAID-M 100) were used to determine the detection range of TDI. 2,4-TDI (CAS: 584-84-9) and HDI (CAS: 822-06-0) were purchased from Sigma Aldrich GmbH (Steinheim, Germany). For preparation of a calibration curve, 2,4-TDI was diluted in pentane (50 ng μl^{-1}). To achieve different gas concentrations, defined volume rates (43 $\mu\text{l h}^{-1}$ to 560 $\mu\text{l h}^{-1}$) of the TDI solution were injected via a syringe pump into a clean air flow (60 l h^{-1}). Air was cleaned by means of an activated charcoal filter prior to the introduction of the sample. Spectra were acquired using Bruker IMS software; XIMS PLUS 1.0. HDI was measured similarly.

Results

Bruker's IMS devices were capable of rapidly detecting TDI/HDI down to 1 ppb (0.007 mg m^{-3}), which is below the lower limit of common workplace exposure limits (Tab.1). The introduction of TDI to the IMS devices resulted in a single substance-specific signal in negative polarity at a drift time of 13.12 ms (reduced drift time of 1.46 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, cf. Fig.1).

Table 1: Overview of occupational exposure limits

Occupational exposure limits for 2,4-TDI and HDI [1, 2]			
Agency/ Association	Workplace Limits	TDI [ppm]	HDI [ppm]
Occupational Safety and Health Administration (OSHA)	PEL ¹	0.02	n.e.
American Conference of Governmental Industrial Hygienists (ACGIH)	TLV ² -TWA ³	0.001	0.005
	TLV-STE ⁴	0.005	0.02
National Institute for Occupational Safety and Health (NIOSH)	REL ⁵	n.e.	0.005
	IDLH ⁶	2.5	n.d.
Deutsche Gesetzliche Unfallversicherung (DGUV)	AGW ⁷	0.005	0.005

¹PEL ... Permissible Exposure Limits

²TLV ... Threshold Limited Value

³TWA ... Time Weighted Average

⁴STE⁴ ... Short-Term Exposure Limits

⁵REL ... Recommended Exposure Limits

⁶IDLH ... Immediately Dangerous to Life or Health

⁷AGW ... Arbeitsplatzgrenzwert (Workplace Exposure Limit in Germany)

n.d. ... not defined

n.e. ... not established

2,4-TDI and 2,6-TDI show identical results. The introduction of the HDI resulted in two peaks: one in positive polarity ($K_0 = +1.40$) and one in negative polarity ($K_0 = -1.41$).

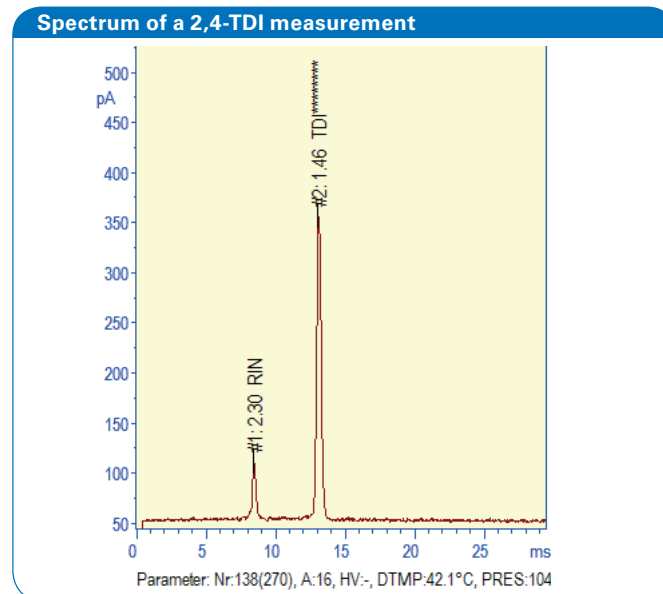


Figure 1: Spectrum of a 2,4-TDI measurement showing one peak for TDI and the reactant ion peak negative (RIN).

The resulting peak systems enabled the detection of TDI and HDI in approximately 5 seconds. In autonomous mode, the instrument software identifies TDI and HDI automatically based on this substance-specific ion peaks. For a quantitative output, an integrated bar reading (web interface or instrument display) can be used. One to eight bars correspond to specific concentration areas.

Conclusion

The stationary device TIMON is best suited for 24/7 ambient air monitoring at workplaces, because of their low maintenance requirements and service intervals. However, the handheld detector RAID-M 100 enables identifying source of leaks, monitoring transportation and filling processes as well as providing information in case of disasters.

References

- [1] OSHA Chemical Sampling Information. <https://www.osha.gov>
- [2] Technical Rule for Hazardous Substances (TRGS 900: AGW). <http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/TRGS/TRGS-900.html> (accessed October 28, 2015).



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