



# **GAS DETECTION LIMITS**

Highly Accurate, Reliable, and Stable Gas Monitoring





## About LumaSense Technologies

LumaSense Technologies, an Advanced Energy Company, enables customers worldwide to achieve predictable and sustainable improvements in process efficiency and waste reduction. These customers have processes that include generating and transmitting electricity; oil and gas refining; processing industrial materials like steel and glass; and manufacturing advanced technologies such as semiconductor, wafers, and LEDs.

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Our gas portfolio consists of gas modules and instruments that provide superior sensitivity over other gas detection techniques. Photoacoustic Spectroscopy (PAS) gas instruments were pioneered and perfected by Innova®. Microphone technology is an important tool in measuring gases through the use of PAS and this is a unique technique offering

the customer an outstanding degree of measurement stability with exceptional sensitivity. Our engineering team continually works to improve the PAS technique and to test its applications in new areas. With PAS, the absorption (proportional to the concentration) is measured directly and not relative to a background, making PAS highly accurate and stable.

## Detection limits of Innova gas-monitors from LumaSense using various optical filters

Since most gases have characteristic infrared absorption spectra, infrared spectroscopy is an excellent monitoring tool. LumaSense has a selection of Innova monitors exploring this technique – Infrared Photo Acoustic Spectroscopy (PAS) to provide very stable and sensitive gas monitors.

The selectivity of any infrared detection method is enhanced by selective irradiation with light of the desired wavelength. The range of optical filters is designed to provide the best options for choosing the optimal light wavelength range for the specific monitoring need.

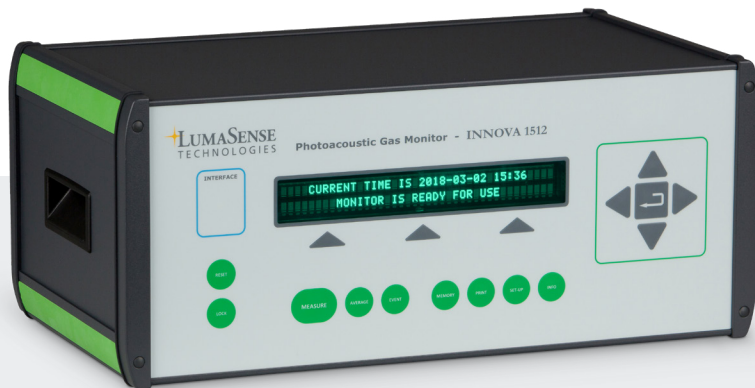
Photoacoustic Gas Monitor – Innova 1512 is capable of simultaneous monitoring up to five component gases and water vapor in any air sample. The monitor is well suited and very efficient in both short and long term monitoring applications. In short term monitoring, the benefit is portability, the minimal warm-up time, and built-in data storage capability. In long term monitoring, the PAS system is especially stable, includes a multi-point sampling option, and data handling.

The Innova 1512 can be configured to perform almost any kind of monitoring task. A special optical filter is permanently installed and enables water vapor contribution

to be measured separately during each measurement cycle. The instrument is then able to compensate for water vapor interference. Any other gas, which is known to be present in the ambient air, can be compensated for in a similar way. By installing an optical filter to selectively measure the concentration of the interfering gas, the user can set up the 1512 to compensate for the interfering gas' contribution.

The Photoacoustic Gas Monitor – Innova 1314i has the same specifications as the 1512 instrument, but it is housed in a rugged box that fits in a standard 19 inch rack.

Included with the 1512 and the 1314i is user software. The software displays measurement data in a table or a graphical window and it uses a SQL Server 2014 database giving online access to measurement data from Microsoft® Excel.



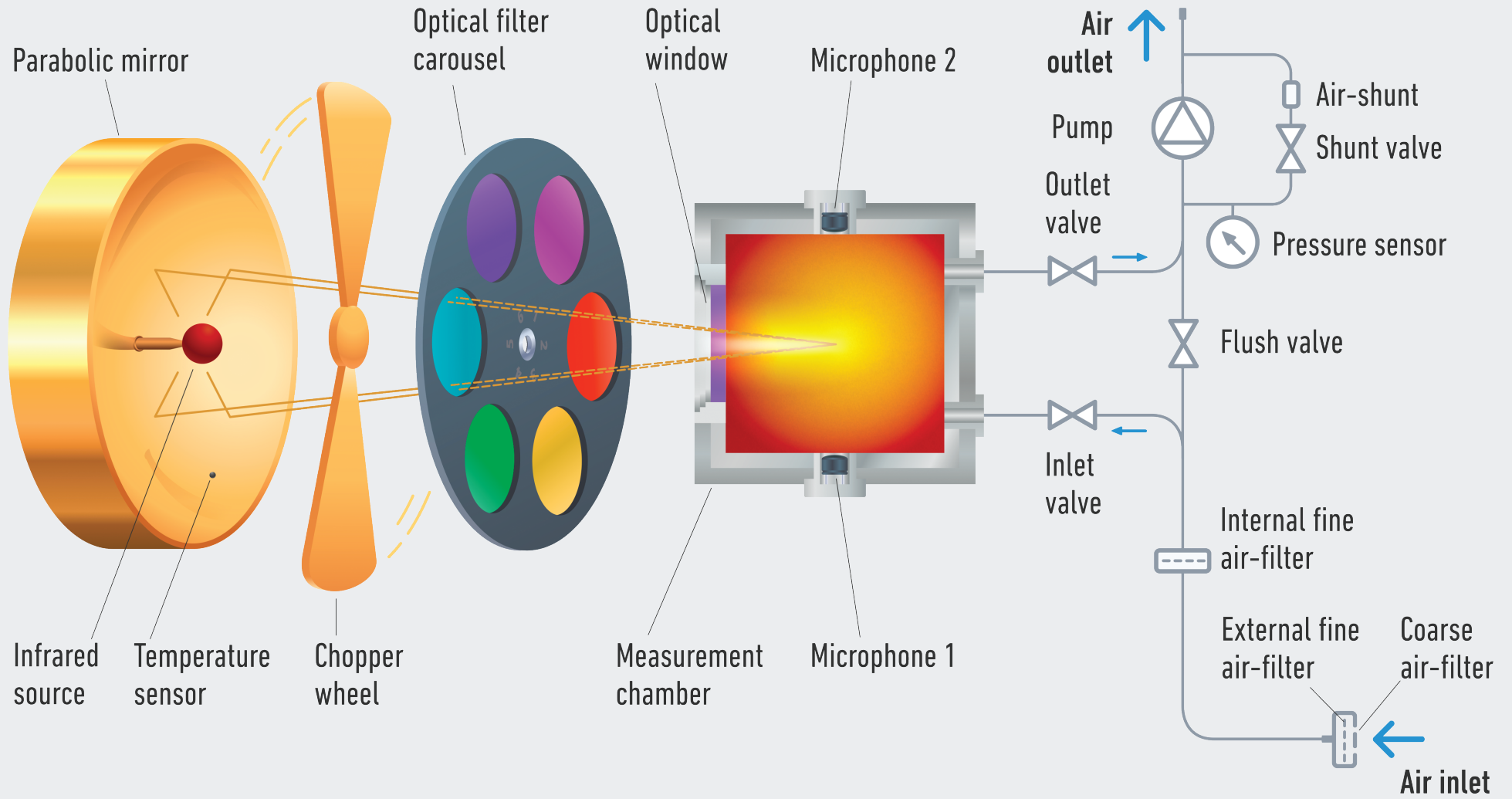
PHOTOACOUSTIC GAS MONITOR – INNOVA 1512



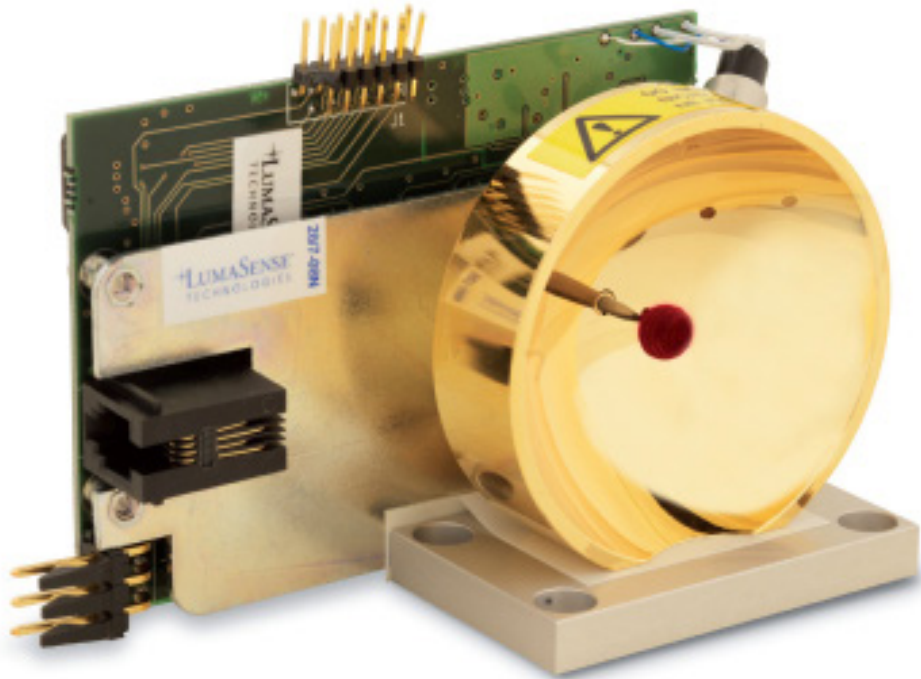
PHOTOACOUSTIC GAS MONITOR – INNOVA 1314i

# Photoacoustic Spectroscopy (PAS)

PAS system used in the Innova instruments







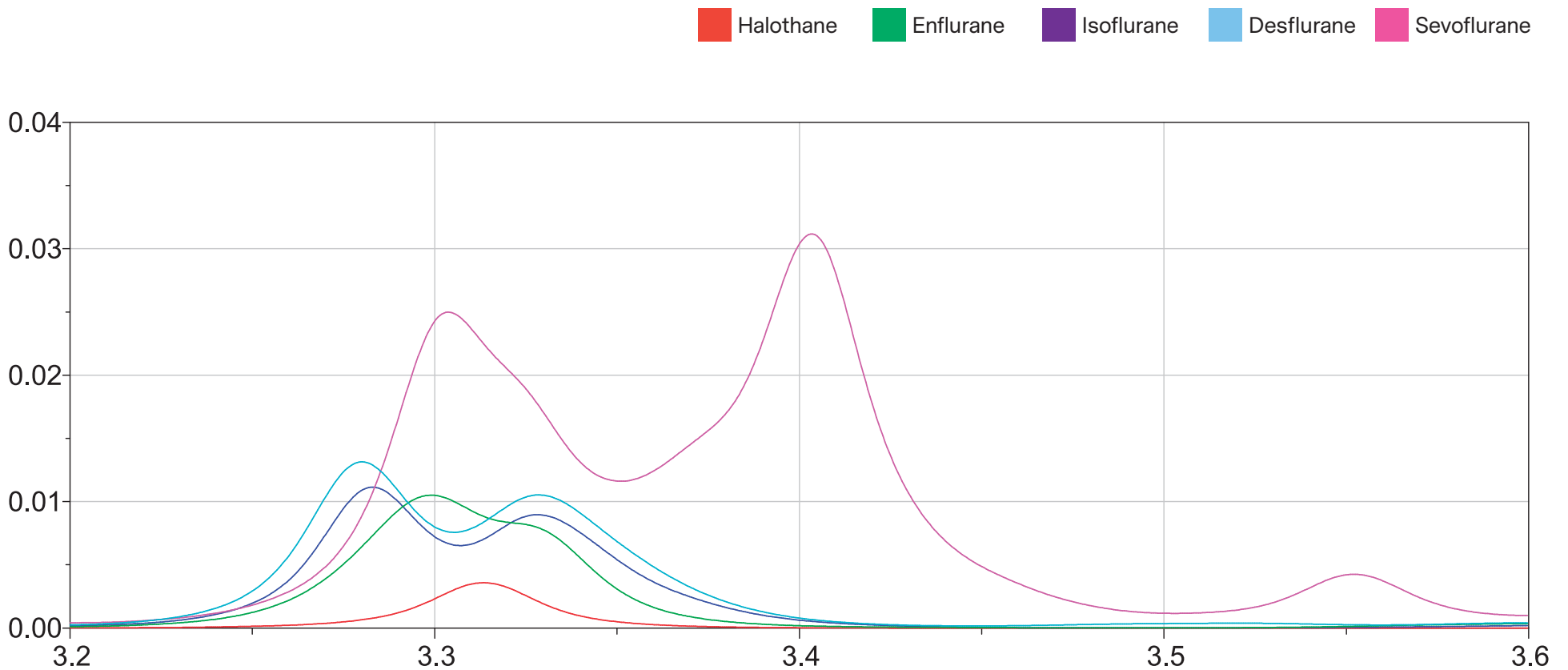
UNIT OF IR-SOURCE WITH ELLIPSOID MIRROR



UNIT OF PAS MEASUREMENT CELL

## Infrared spectra

The  $\rightarrow$  C – H fundamental stretching vibration frequencies are always in the region from 3.2 to 3.6  $\mu\text{m}$ . The infrared spectra for Halothane, Enflurane, Isoflurane, Desflurane, Sevoflurane in that region is shown in the figure below.



# The optical filters

Optical filters used in Innova instruments display different characteristics, while sharing a basic design.

Each filter comprises three separate infrared elements; a narrow-band pass element, a short-wave pass element and a wide-band pass element. The narrow-band pass element has very specific transmission characteristics. These are further defined by short-wave pass and wide-band pass elements, which prevent transmission of light at other wavelengths; as a result the optical filters have low leakage characteristics.

The narrow-band pass filter determines the center wavelength and bandwidth of the optical filter, and, thus, which gases can be detected. The ranges of optical filters span the entire “fingerprint” region (700 to 1350 cm<sup>-1</sup>) plus the region between 2000 and 3000 cm<sup>-1</sup> (see Fig. 1 and Table 1). The “gap” in the infrared spectrum between 1350 cm<sup>-1</sup> and 2000 cm<sup>-1</sup> is due to strong water absorption. This region is only suited for monitoring water vapor.

In the Table 1 the specifications for the 27 optical filters is summarized. The bandwidth is given as a percentage of the filter center wavelength.

For example, the bandwidth of UA0987 becomes 3.4µm x 6,0% = 0.204µm.

All LumaSense optical filters comply with MIL-SC-48497A requirements.

## Fig. 1 and Table 1 contain 4 special filters

SB0527 is the standard filter for measurement of water vapor. The detection limit for this filter is 50 ppm.

UA6010 is a high sensitive filter for measurement of water vapor. The detection limit for this filter is 0.1 ppm. The main application is measurement of humidity in pure gases.

UA6009 is a high sensitive filter for measurement of carbon dioxide. The detection limit for this filter is 7 ppb. The main application is measurement of carbon dioxide in pure gases.

UA6008 is a dedicated filter for measurement of mustard gas. The detection limit for this filter is 0.1 ppm.

## Choosing a filter

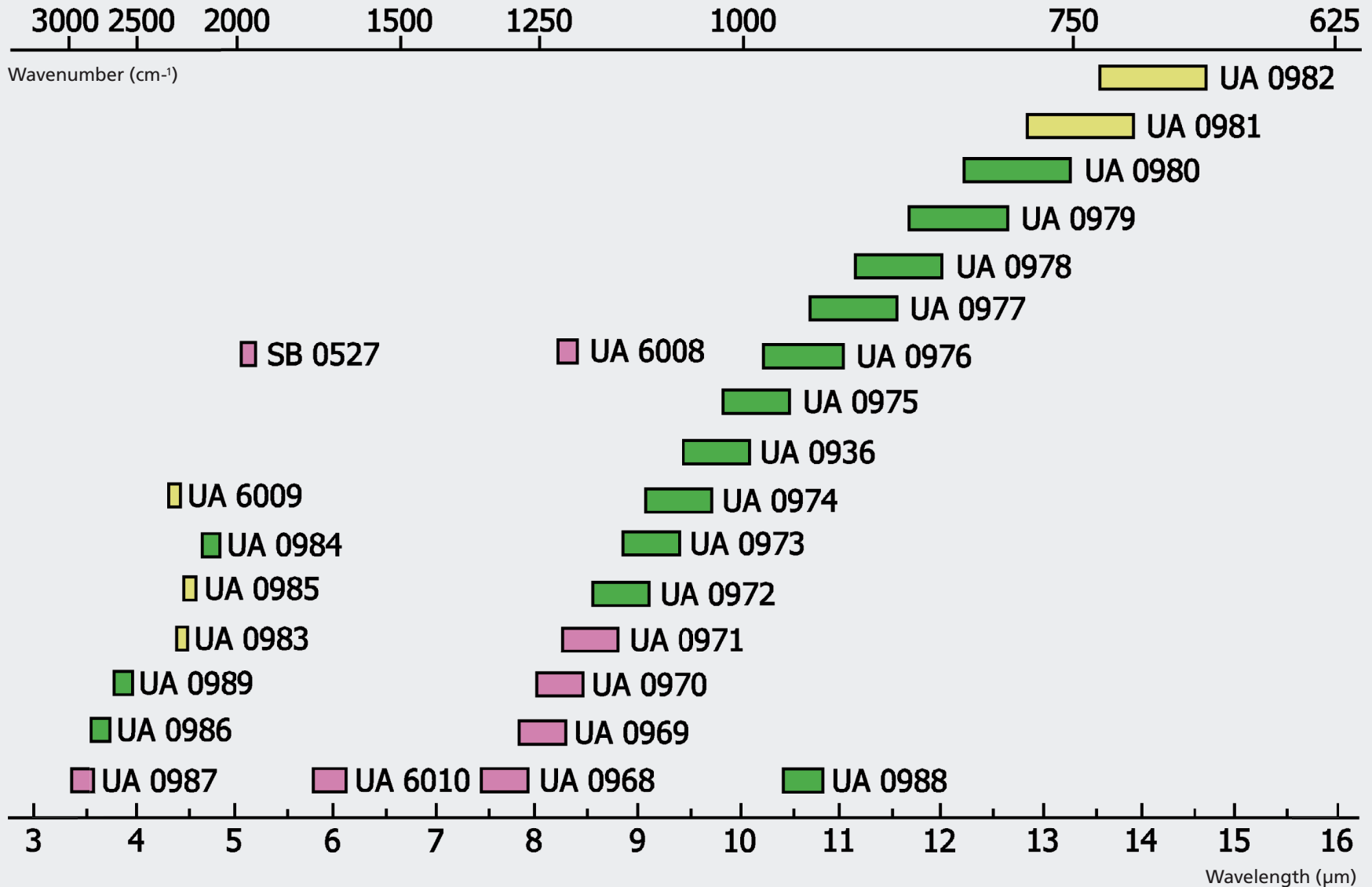
Immunity to interfering species is perhaps the most important consideration in any gas detection application. Careful consideration of potential interference is therefore essential. Depending on the concentration and type of interfering gases and on the measurement range required, different filters may be selected in different applications in order to measure the same gas.

Optical Filter Number	Filter Centre µm	Filter Centre cm <sup>-1</sup>	Bandwidth %
UA0987	3.4	2950	6
UA0986	3.6	2800	3
UA0989	3.6	2750	1.5
UA6009	4.3	2347	2
UA0983	4.4	2270	1.3
UA0985	4.5	2215	2
UA0984	4.7	2150	3
SB0527	5.1	1985	2
UA6010	5.9	1700	5.9
UA0968	7.7	1291	5.5
UA0969	8	1254	5.5
UA0970	8.2	1217	5.5
UA6008	8.3	1210	3
UA0971	8.5	1179	6
UA0972	8.8	1139	6
UA0973	9.1	1101	6
UA0974	9.4	1061	6.5
UA0936	9.8	1020	6.5
UA0975	10.2	981	6.5
UA0976	10.6	941	7
UA0988	10.6	946	3.7
UA0977	11.1	900	7
UA0978	11.6	861	7
UA0979	12.2	822	7.5
UA0980	12.8	783	7.5
UA0981	13.4	746	7.5
UA0982	14.1	710	7.5

Dimensions	
Diameter	31.00 mm
Height	5.15 mm
Operating Temperature	-20°C to +70°C
Relative Humidity	0% to 95% RH
Storage Temperature	-25°C to +70°C

# Wavenumber/wavelength and bandwidth

Fig. 1 Center wavelength and half-power bandwidths of the optical filters





# Information about this chart

For each gas/vapor in the table below, one or more optical filters and corresponding detection limits are listed.

The interference caused by water vapor and carbon dioxide in ambient air is a problem inherent in all infrared methods of detection. The extent of this interference is dependent on the optical filter used. Some optical filters are more sensitive to these substances than others, and color-coding has been introduced to illustrate the sensitivity of the filters (details are given below).

## Color coding of the optical filters used in the chart

### These optical filters are sensitive to water vapor.

In these regions of the infrared spectrum, water vapor interferes heavily with all infrared technologies. However, the unique water compensation algorithm of the Innova gas monitors minimizes this effect, thus, expanding the usable range of infrared measurements.

### These optical filters are sensitive to carbon dioxide.

Carbon dioxide interference can, however, be compensated for when using the 1512 and 1314i instruments. An optical filter can be installed in the monitors to measure the level of carbon dioxide and the instruments can then automatically compensate for the interference.

### These optical filters are not affected by interference from carbon dioxide and water vapor.

If a gas is measured in clean ambient air using one of these optical filters, the listed detection limit will not be affected by the presence of carbon dioxide or water vapor, except if these are present in very high concentrations.

**Detection limit:** The minimum concentration of a substance that produces an observable response. For the Innova gas monitors, the an "observable response" is equal to twice the noise signal on the measured concentrations when monitoring in dry air.

**Sample Integration Time (SIT):** To optimize each measurement task, providing faster response time or lower detection limits, the Photoacoustic Gas Monitor – Innova 1512 and the Photoacoustic Gas Monitor – Innova 1314i have the option of adjusting the SIT between 0.5 and 50 seconds.

SIT	0.5	1	2	5	10	20	50
DLF	3.2	2.2	1.6	1.0	0.7	0.5	0.3

The DLF is the Detection Limit Factor. To get the detection limit at a given SIT one has to multiply the detection limit in the chart with the corresponding DLF:

$$Detection\ limit = Detection\ limit\ in\ chart \times DLF$$

For more information look at the example on the back of this chart.

**Dynamic range:** The 1512 and 1314i instruments have very wide dynamic ranges of up to five orders of magnitude. This means that the measurement range is from the detection limit of a gas up to 100,000 times the detection limit at 5 SIT.

**Note:** This chart should only be used as a guide when choosing an optical filter for a specific measurement task. If more than one infrared absorbing gas is present in the air being monitored, this will frequently affect the choice of optical filter. Consequently, it is recommended that the local LumaSense representative is contacted for help in choosing the optimum filter configuration.

Notification used in the chart:

  = Measured detection limit verified by LumaSense laboratory

Normal = Calculated detection limit

Relative strenght of absorption band:

vw = very weak      s = strong  
 w = weak            vs = very strong  
 m = medium

Detection limits in part per million at 20°C, 1 atmosphere pressure and SIT=5 sec.			Optical filter number																							
			Centre wavelength (in micrometer) Centre wavenumber (in cm <sup>-1</sup> )																							
Name	Brutto- formula	Molec.- weight	987 3.4 2950	986 3.6 2800	989 3.7 2750	983 4.4 2270	985 4.5 2215	984 4.7 2150	968 7.7 1291	969 8.0 1254	970 8.2 1217	971 8.5 1179	972 8.8 1139	973 9.1 1101	974 9.4 1061	936 9.8 1020	975 9.8 981	988 10.6 946	976 10.6 941	977 11.1 900	978 11.6 861	979 12.2 822	980 12.8 783	981 13.4 746	982 14.1 710	
Acetaldehyde	C <sub>2</sub> H <sub>4</sub> O	44.05	0.1	0.08	0.2								0.2	0.2												
Acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.05									0.04	0.03														
Acetic anhydride	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	102.09								0.04					0.05					0.1						
Acetone	C <sub>3</sub> H <sub>6</sub> O	58.08	0.1							0.07	0.06															
Acetonitrile	C <sub>2</sub> H <sub>3</sub> N	41.05	w		w										2.5	w				w						
Acetylene	C <sub>2</sub> H <sub>2</sub>	26.04								1													0.3	0.3	0.3	
Acrolein	C <sub>3</sub> H <sub>4</sub> O	56.06	0.1	0.1	m								0.2			0.09			0.1							
Acrylonitrile	C <sub>3</sub> H <sub>3</sub> N	53.06														0.3	0.2		0.2							
Allyl chloride	C <sub>3</sub> H <sub>5</sub> Cl	76.52	0.2							0.2									0.2						0.4	
Ammonia	NH <sub>3</sub>	17.03												0.2			0.2		0.2							
Aniline	C <sub>6</sub> H <sub>7</sub> N	93.13	0.3							0.09					0.2										0.2	
Arsine	AsH <sub>3</sub>	77.95					0.05	0.03									0.4		0.4							
Benzaldehyde	C <sub>7</sub> H <sub>6</sub> O	106.12		0.07								0.09													0.3	
Benzene	C <sub>6</sub> H <sub>6</sub>	78.11	0.1												0.9	0.8	21								0.3	
Benzyl chloride / α-Chlorotoluene	C <sub>7</sub> H <sub>7</sub> Cl	126.58	0.1							0.1															0.3	0.1
Biphenyl	C <sub>12</sub> H <sub>10</sub>	154.21	m																	w						
Boron trifluoride	BF <sub>3</sub>	67.81														0.2									0.07	
Bromoform / Tribromomethane	CHBr <sub>3</sub>	252.73	vw									0.1	0.06	12												1
Bromomethane	CH <sub>3</sub> Br	94.94	0.2						0.5																	
1,3-Butadiene	C <sub>4</sub> H <sub>6</sub>	54.09	0.2													0.2			0.1	0.2						
Butane	C <sub>4</sub> H <sub>10</sub>	58.12	0.01	0.5																						
Butane-2,3-dione	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	86.09											0.06	0.06												
Butanethiol / Butyl mercaptan	C <sub>4</sub> H <sub>10</sub> S	90.19	s							s													m			
1-Butanol	C <sub>4</sub> H <sub>10</sub> O	74.12	0.01							0.2					0.08				0.5							
2-Butanol	C <sub>4</sub> H <sub>10</sub> O	74.12	s										m			m				m						
tert-Butanol / tert-Butyl alcohol	C <sub>4</sub> H <sub>10</sub> O	74.12	0.03										0.08							0.2						
2-Butanone / Methyl ethyl ketone(MEK)	C <sub>4</sub> H <sub>8</sub> O	72.11	0.04	1							0.2	0.07							0.5							
2-Butenal / Crotonaldehyde	C <sub>4</sub> H <sub>6</sub> O	70.09	m	m	s								s	0.2				s								
2-Butoxyethanol	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	118.17	0.01									0.05	0.04									0.4				
n-Butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	0.02							0.01				0.08	0.05											
sec-Butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	s							s				s				m								
tert-Butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	s							s		s														
Butyl acrylate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	128.17	0.02	0.02							0.02			0.09												
tert-Butyl alcohol / tert-Butanol	C <sub>4</sub> H <sub>10</sub> O	74.12	0.03										0.08							0.2						
Butyraldehyde	C <sub>4</sub> H <sub>8</sub> O	72.11	s	s																					1	
Butyric acid	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.11	0.04										0.04	0.06												
Carbon dioxide	CO <sub>2</sub>	44.01				5	70																	13	1.5	
Carbon disulfide	CS <sub>2</sub>	76.14					1	0.6																		
Carbon monoxide	CO	28.01					0.5	0.2																		
Carbonyl chloride / Phosgene	COCl <sub>2</sub>	98.92																				0.02	0.02			
Carbonyl sulfide	COS	60.08	0.3					1														0.6				
Chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	112.56												0.09	0.2											0.2
2-Chloroethyl ether	C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O	143.01	0.03	0.4						0.4			0.02	0.02												
Chloroform	CHCl <sub>3</sub>	119.38									0.09												0.3	0.04		
Chloromethane	CH <sub>3</sub> Cl	50.49	0.2													2									0.6	
1-Chloro-1-nitropropane	C <sub>3</sub> H <sub>6</sub> ClNO <sub>2</sub>	123.54	m							m								m			m					
α-Chlorotoluene / Benzyl chloride	C <sub>7</sub> H <sub>7</sub> Cl	126.58	0.1							0.1															0.3	0.1
m-Cresol / 3-Methylphenol	C <sub>7</sub> H <sub>8</sub> O	108.14	0.07								0.05								0.3						0.3	
Crotonaldehyde / 2-Butenal	C <sub>4</sub> H <sub>6</sub> O	70.09	m	m	s									0.2				s								

Name	Brutto-formula	Molec.-weight	987 3.4 2950	986 3.6 2800	989 3.7 2750	983 4.4 2270	985 4.5 2215	984 4.7 2150	968 7.7 1291	969 8.0 1254	970 8.2 1217	971 8.5 1179	972 8.8 1139	973 9.1 1101	974 9.4 1061	936 9.8 1020	975 10.2 981	988 10.6 946	976 10.6 941	977 11.1 900	978 11.6 861	979 12.2 822	980 12.8 783	981 13.4 746	982 14.1 710
Cumene / Isopropylbenzene	C <sub>9</sub> H <sub>12</sub>	120.19	m											m		0.7							m		
Cyanogen / Isocyan	C <sub>2</sub> N <sub>2</sub>	52.03					1.1	0.6																	
Cyanogen bromide	BrCN	105.92					0.1																		
Cyanogen chloride	CNCl	61.47					0.3	0.4																	
Cyclohexane	C <sub>6</sub> H <sub>12</sub>	84.16	0.008	0.2						0.7															
Cyclohexanone	C <sub>6</sub> H <sub>10</sub> O	98.14	s								0.2										m				
Cyclohexene	C <sub>6</sub> H <sub>10</sub>	82.14	0.02																		0.9				
Cyclopentane	C <sub>5</sub> H <sub>10</sub>	70.1	vs	0.7														m							
n-Decane	C <sub>10</sub> H <sub>22</sub>	142.28	0.007						0.3																
1-Decene	C <sub>10</sub> H <sub>20</sub>	140.27	0.009						0.3										0.3						
Desflurane	C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O	168.04								0.005		0.008													m
Deuterium oxide	D <sub>2</sub> O	20.03		0.3						s				s											
Diamine / Hydrazine	N <sub>2</sub> H <sub>4</sub>	32.05													0.6	0.6					0.6				
Diaminoethane	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	60.10	0.04											0.7									0.1		
Diborane	B <sub>2</sub> H <sub>6</sub>	27.67									0.1	0.1													
o-Dichlorobenzene / 1,2-Dichlorobenzene	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.00	4												0.3										0.1
m-Dichlorobenzene / 1,3-Dichlorobenzene	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.00	2											0.1									0.1	0.15	
p-Dichlorobenzene / 1,4-Dichlorobenzene	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	147.00												0.05	0.2							0.2			
1,1-Dichloroethane	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	98.96	0.2								0.2				0.1										0.09
1,2-Dichloroethane	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	98.96	0.2							0.1															0.3
1,1-Dichloroethene	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.94												vs								0.09			m
1,2-Dichloroethene (cis)	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.94						0.2													0.09	0.2			s
1,2-Dichloroethene (trans)	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	96.94									0.2										0.07	0.05			
Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	84.93	0.6								0.5												0.1	0.08	
1,1-Dichloro-1-nitroethane	C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> NO <sub>2</sub>	143.96													m						m				m
1,2-Dichloropropane	C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub>	112.99	0.08								0.3					0.3									0.5
Diethylamine	C <sub>4</sub> H <sub>11</sub> N	73.14	0.02									0.1													0.4
2-(Diethylamino)-ethanol	C <sub>8</sub> H <sub>15</sub> NO	117.19	s								m				0.4										
Diethylen glycol dimethyl ether	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>	134.17	0.01									0.02	0.02												
Diethylen glycol butyl ether	C <sub>8</sub> H <sub>18</sub> O <sub>3</sub>	162.23	s	m										s	s						m				
Diethylentriamin	C <sub>4</sub> H <sub>13</sub> N <sub>3</sub>	103.17	s		0.4						0.4				0.3							0.3			
Diethyl ether	C <sub>4</sub> H <sub>10</sub> O	74.12	0.02									0.02	0.08												
Diethyl ketone (DEK) / 3-Pentanone	C <sub>5</sub> H <sub>10</sub> O	86.13	0.01										0.1							0.2					
N,N-Dimethyl acetamide	C <sub>4</sub> H <sub>9</sub> NO	87.12	m								m					0.3	0.2								
Dimethylamine (DMA)	C <sub>2</sub> H <sub>7</sub> N	45.08	0.02	0.04								0.1											0.3		
2-(Dimethylamino)-ethanol	C <sub>4</sub> H <sub>11</sub> NO	89.14	s											vs							m				
N,N-Dimethylanilin	C <sub>8</sub> H <sub>11</sub> N	121.18	m								m					m									m
Dimethyl disulfide	C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	94.20	s						s									0.6							
Dimethyl ester sulfuric acid (DMS)	C <sub>2</sub> H <sub>6</sub> O <sub>4</sub> S	126.13	0.07													0.02	0.06					0.05			
Dimethylether	C <sub>2</sub> H <sub>6</sub> O	46.07	s									0.07		0.2											
Dimethylethylamine	C <sub>4</sub> H <sub>11</sub> N	73.14	s								0.2			0.2									0.8		
Dimethylformamide (DMF)	C <sub>3</sub> H <sub>7</sub> NO	73.09	0.1								0.3			0.06	0.07		3								0.9
2,6-Dimethyl-4-heptanone	C <sub>9</sub> H <sub>18</sub> O	142.24	0.008							0.5				0.3											
1,1-Dimethylhydrazine	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	60.10	s												s					s					
Dimethylnitrosamine	C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O	74.08	0.04							0.06						0.03									
Dimethyl sulfoxide	C <sub>2</sub> H <sub>6</sub> OS	78.13	0.3											0.07		0.6									
Dimethyl sulfate	C <sub>2</sub> H <sub>6</sub> O <sub>4</sub> S	126.13	m								s					vs						0.06			
Dimethyl sulfide	C <sub>2</sub> H <sub>6</sub> S	62.13	s	0.4											0.7	0.6									
Dimethyl sulfite	C <sub>2</sub> H <sub>6</sub> O <sub>3</sub> S	110.13	m								s						s							m	
Dinitrogen difluoride	N <sub>2</sub> F <sub>2</sub>	66.01															0.02	0.2							
Dinitrogen oxide / Nitrous Oxide	N <sub>2</sub> O	44.01					0.03	0.5																	
1,4-Dioxane / 1,4-Diethylene oxide	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.11	0.02										0.02								0.07				

Name	Brutto-formula	Molec.-weight	987 3.4 2950	986 3.6 2800	989 3.7 2750	983 4.4 2270	985 4.5 2215	984 4.7 2150	968 7.7 1291	969 8.0 1254	970 8.2 1217	971 8.5 1179	972 8.8 1139	973 9.1 1101	974 9.4 1061	936 9.8 1020	975 10.2 981	988 10.6 946	976 10.6 941	977 11.1 900	978 11.6 861	979 12.2 822	980 12.8 783	981 13.4 746	982 14.1 710	
Diphenyl ether	C <sub>12</sub> H <sub>10</sub> O	170.21	m/w							s	s									s						
Dipropylnitrosamine	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O	130.19	0.03									0.1			0.05											
Enflurane	C <sub>3</sub> H <sub>2</sub> ClF <sub>5</sub> O	184.49	0.1									0.007	0.005										0.08			
Epichlorohydrin	C <sub>3</sub> H <sub>5</sub> ClO	92.52	m										0.9									0.2				
Ethane	C <sub>2</sub> H <sub>6</sub>	30.07	0.02																				1			
Ethanethiol / Ethyl mercaptan	C <sub>2</sub> H <sub>6</sub> S	62.13	s														1		2							
Ethanol	C <sub>2</sub> H <sub>6</sub> O	46.07	0.03										0.2		0.08	0.08										
Ethanolamine	C <sub>2</sub> H <sub>7</sub> NO	61.08	0.09												0.1								0.7			
Ethene	C <sub>2</sub> H <sub>4</sub>	28.05	0.3														0.2				0.4					
2-Ethoxyethanol / Cellosolve	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	90.12	s										0.02		s				m							
2-Ethoxy ethylacetate	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	132.16	0.02						0.02		0.01									0.3						
Ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.11	0.03							0.01					0.05								0.8			
Ethyl acrylate	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	100.12	0.04									0.02			0.06					0.2						
Ethylamine	C <sub>2</sub> H <sub>7</sub> N	45.08												0.2									0.07	0.09		
Ethyl benzene	C <sub>8</sub> H <sub>10</sub>	106.17	0.01												0.5									0.4	0.09	
Ethylene glycol / Ethanediol	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	62.07	m											0.08	0.05							m				
Ethylene oxide	C <sub>2</sub> H <sub>4</sub> O	44.05	0.08						0.3											0.2	0.1					
Ethyl formate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.08	0.03									0.03				0.4										
2-Ethyl-1-Hexanol	C <sub>8</sub> H <sub>18</sub> O	130.23	0.008												0.08		0.3									
Ethylhexyl acrylate	C <sub>11</sub> H <sub>20</sub> O <sub>2</sub>	184.28	s									0.03				m				0.4						
5-Ethyl-2-methylpyridine	C <sub>8</sub> H <sub>11</sub> N	121.18	s													m						0.6				
Fluorobenzene	C <sub>6</sub> H <sub>5</sub> F	96.10	7							0.03														0.2		
Formaldehyde	CH <sub>2</sub> O	30.03	0.1	0.04	0.1																					
Formic acid	CH <sub>2</sub> O <sub>2</sub>	46.03	0.01								0.2		0.04	0.02												
Freon 11 / Trichlorofluoromethane	CCl <sub>3</sub> F	137.37													0.04	0.04						0.02				
Freon 12 / Dichlorodifluoromethane	CCl <sub>2</sub> F <sub>2</sub>	120.91										0.02	0.02								0.03					
Freon 12B2 / Dibromodifluoromethane	CB <sub>2</sub> F <sub>2</sub>	209.82												0.08	0.1								0.1			
Freon 13 / Chlorotrifluoromethane	CClF <sub>3</sub>	104.46									0.02	0.04		0.05												
Freon 14 / Tetrafluoromethane	CF <sub>4</sub>	88.00								0.004	0.08															
Freon 21 / Dichlorofluoromethane	CHCl <sub>2</sub> F	102.92	vw												0.01								0.02			
Freon 22 / Chlorodifluoromethane	CHClF <sub>2</sub>	86.47	0.3										0.02	0.01									0.2			
Freon 23 / Trifluoromethane	CHF <sub>3</sub>	70.01	m										0.007													
Freon 32 / Difluoromethane	CH <sub>2</sub> F <sub>2</sub>	52.02											0.04	0.01	0.03											
Freon 112 / 1,1,2,2-Tetrachloro-1,2-difluoroethane	C <sub>2</sub> Cl <sub>4</sub> F <sub>2</sub>	203.83											s	s		s					s					
Freon 113 / 1,1,2-Trichloro-1,2-trifluoroethane	C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub>	187.38	0.4										0.02	0.02		0.03							0.04			
Freon 114 / 1,2-Dichlorotetrafluoroethane	C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub>	170.92									0.01		0.01													
Freon 115 / Chloropentafluoroethane	C <sub>2</sub> ClF <sub>5</sub>	154.47										0.001		0.003			0.001									
Freon 116 / Hexafluoroethane	C <sub>2</sub> F <sub>6</sub>	138.01								0.01				0.02												
Freon 134a / Tetrafluoroethane	C <sub>2</sub> H <sub>2</sub> F <sub>4</sub>	102.03	0.05									0.01	0.04								0.2					
Freon 141b/1,1-Dichloro-1-fluoroethane	C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> F	116.95															0.6						0.1			
Freon 152 / 1,2-Difluoroethane	C <sub>2</sub> H <sub>4</sub> F <sub>2</sub>	66.05	0.08										0.002							0.09						
Freon152a / 1,1-Difluoroethane	C <sub>2</sub> H <sub>4</sub> F <sub>2</sub>	66.05	vw									0.05	0.01													
Freon 160 / Chloroethane	C <sub>2</sub> H <sub>5</sub> Cl	64.51	0.06							0.2							0.4									
Freon 227 / 1,1,1,2,3,3,3-Heptafluoropropane	C <sub>3</sub> HF <sub>7</sub>	170.03								0.005	0.007		0.01													
Freon 1113 / Chlorotrifluoroethene	C <sub>2</sub> ClF <sub>3</sub>	116.47								0.07						0.04										
Freon 404a														0.2			0.1									
Furfural	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	96.08		0.2												0.1							0.2			
Furfuryl alcohol	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	98.10	m										s				0.1							s		
Glutaraldehyde	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	100.12		0.2	0.06																		0.7			
Halothane	C <sub>2</sub> HBrClF <sub>3</sub>	197.38	0.9									0.02	0.02									0.09				
1,1,1,2,3,3,3-Heptafluoropropane	C <sub>3</sub> HF <sub>7</sub>	170.03								0.005	0.007		0.02													
n-Heptane	C <sub>7</sub> H <sub>16</sub>	100.20	0.009	0.4																						



Name	Brutto-formula	Molec.-weight	987 3.4 2950	986 3.6 2800	989 3.7 2750	983 4.4 2270	985 4.5 2215	984 4.7 2150	968 7.7 1291	969 8.0 1254	970 8.2 1217	971 8.5 1179	972 8.8 1139	973 9.1 1101	974 9.4 1061	936 9.8 1020	975 10.2 981	988 10.6 946	976 10.6 941	977 11.1 900	978 11.6 861	979 12.2 822	980 12.8 783	981 13.4 746	982 14.1 710	
2-Heptanone	C <sub>7</sub> H <sub>14</sub> O	114.19	0.01	0.2								0.3														
3-Heptanone	C <sub>7</sub> H <sub>14</sub> O	114.19	m											m		m										
Hexachloroethane	C <sub>2</sub> Cl <sub>6</sub>	236.74																						s		
Hexafluorobenzene	C <sub>6</sub> F <sub>6</sub>	186.05														0.01	0.02									
Hexanal	C <sub>6</sub> H <sub>12</sub> O	100.16	0.02	m	s			0.2																		
n-Hexane	C <sub>6</sub> H <sub>14</sub>	86.18	0.009	0.1							0.2															
Hexanoic acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	s									m						m								
Hexanol	C <sub>6</sub> H <sub>14</sub> O	102.17	0.02												s	s										
1-Hexene	C <sub>6</sub> H <sub>12</sub>	84.16	0.01																		0.2					
HFO-1233zd / 1-Chloro-3,3,3-trifluoropropene	C <sub>3</sub> H <sub>2</sub> ClF <sub>3</sub>	130.49										0.01	0.009									0.07				
HFO 1234yf / 2,3,3,3-Tetrafluoropropene	C <sub>3</sub> H <sub>2</sub> F <sub>4</sub>	114.04								vs		0.01		0.3						0.2						
HFO 1234ze / trans-1,3,3,3-Tetrafluoroprop-1-ene	C <sub>3</sub> H <sub>2</sub> F <sub>4</sub>	114.04											0.05	0.05					0.5							
Hydrazine / Diamine	N <sub>2</sub> H <sub>4</sub>	32.05													0.6	0.6						0.6				
Hydrogenchloride	HCl	36.46		0.4																						
Hydrogencyanide	HCN	27.03																						0.5	0.2	
Hydrogensulfide	H <sub>2</sub> S	34.08								14	22															
4-Hydroxy-4-methyl-2-pentanone	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	s										m							m						
Isobutyl acetate / 2-Methyl-1-propyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.16	s								s					s										
Isobutyl alcohol / 2-Methyl-1-propanol	C <sub>4</sub> H <sub>10</sub> O	74.12	s	m											s					m						
Isoflurane	C <sub>3</sub> H <sub>2</sub> ClF <sub>5</sub> O	184.49	0.3									0.005		0.008								0.1				
Isooctane / 2,2,4 Trimethylpentane	C <sub>8</sub> H <sub>18</sub>	114.23	0.009								0.4	0.5														
Isopentane / 2-Methylbutane	C <sub>5</sub> H <sub>12</sub>	72.15	0.006	0.4																						
Isopropyl acetate / 2-Propyl acetate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.13	m									s			s					m						
Isopropylbenzene / Cumene	C <sub>9</sub> H <sub>12</sub>	120.19	m											m		0.7							m			
Limonene	C <sub>10</sub> H <sub>16</sub>	136.23	0.01																		0.2	0.4				
Maleic anhydride	C <sub>4</sub> H <sub>2</sub> O <sub>3</sub>	98.06									m				m					m						
Methane	CH <sub>4</sub>	16.04	0.1						0.2	0.4																
Methanethiol / Methyl mercaptan	CH <sub>4</sub> S	48.11	0.1											0.9		1										
Methanol	CH <sub>4</sub> O	32.04	0.04								0.5				0.08		0.2									
2-Methoxyethanol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	76.09	m	0.1									0.04	0.05												
Methoxyflurane	C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> F <sub>2</sub> O	164.97	0.05							0.04				0.01								0.03				
1-Methoxy-2-propanol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	90.12	s								0.06		0.02	0.04												
Methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.08	0.04							0.04					0.05											
Methyl acrylate	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	86.09	0.05								0.02			0.1			0.2									
Methylamine	CH <sub>5</sub> N	31.06	0.04	0.2												0.6						0.2				
o-Methylanilin / o-Toluidine	C <sub>7</sub> H <sub>9</sub> N	107.15	0.05							0.1					0.4									0.1		
Methylbiphenyl	C <sub>13</sub> H <sub>12</sub>	168.23	s									m				m							s			
2-Methylbutadien / Isoprene	C <sub>5</sub> H <sub>8</sub>	68.12	0.1																0.4	0.3						
3-Methyl-1-butanol / Isoamyl alcohol	C <sub>5</sub> H <sub>12</sub> O	88.15	s	s											m											
3-Methyl-2-butanone / Methyl isopropyl ketone	C <sub>5</sub> H <sub>10</sub> O	86.13	0.02					0.2											0.5							
3-Methylbutyl acetate / Isoamyl acetate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.19	0.02								0.01					0.1				0.9						
Methyl tert-butyl ether	C <sub>5</sub> H <sub>12</sub> O	88.15	0.01								0.04			0.05												
Methyl chloroformate	C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub>	92.50									0.04	0.01	0.02									0.2				
Methylcyclohexane	C <sub>7</sub> H <sub>14</sub>	98.19	0.01							1																
Methyl formate	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.05	0.03							0.03		0.02									0.3					
4-Methyl-3-heptanone	C <sub>8</sub> H <sub>16</sub> O	128.21	s											m			m									
Methylhydrazine	CH <sub>6</sub> N <sub>2</sub>	46.07	0.07	0.1																0.2			0.3			
Methyl iodide	CH <sub>3</sub> I	141.94	0.3							0.2										1.3						
Methyl isobutyl carbinol / 4-Methyl-2-pentanol	C <sub>6</sub> H <sub>14</sub> O	102.17	s										m		m					m						
Methyl isobutyl ketone(MIBK)/4-Methyl-2-pentanone	C <sub>6</sub> H <sub>12</sub> O	100.16	0.02									0.08							0.1							
Methyl isopropyl ketone / 3-Methyl-2-butanone	C <sub>5</sub> H <sub>10</sub> O	86.13	0.02					0.2											0.5							
Methyl methacrylate	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	100.12	0.04									0.02							0.2				0.6			

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4-Methyl-2-pentanol / Methyl isobutyl carbinol	C <sub>6</sub> H <sub>14</sub> O	102.17	s										m		m						m					
2-Methylpropane / Isobutane	C <sub>4</sub> H <sub>10</sub>	58.12	0.01										0.9													
2-Methylpropene	C <sub>4</sub> H <sub>8</sub>	56.11	0.02																	0.2	0.4					
1-Methyl-2-pyrrolidone / N-Methylpyrrolidone	C <sub>5</sub> H <sub>9</sub> NO	99.13	s						0.04		0.2			0.3												
Methylsalicylate	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	152.15	0.1							0.02	0.03											0.7				
α-Methylstyrene	C <sub>9</sub> H <sub>10</sub>	118.18	m																	s			0.5		s	
2-Methylstyrene	C <sub>9</sub> H <sub>10</sub>	118.18	s														s			m				s		
Monomethylhydrazine	CH <sub>6</sub> N <sub>2</sub>	46.07	s													s			s						m	
Morpholine	C <sub>4</sub> H <sub>9</sub> NO	87.12	m	0.04											0.2									0.2		
Naphthalene	C <sub>10</sub> H <sub>8</sub>	128.17	0.07						0.5														0.06			
Nitrobenzene	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	123.11													0.5							0.3				
Nitroethane	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	75.07	m														m			m						
Nitrogen trifluoride	NF <sub>3</sub>	71.00													0.2			0.1		0.2						
Nitromethane	CH <sub>3</sub> NO <sub>2</sub>	61.04											0.5							0.7						
1-Nitropropane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	89.09	m								m													m		
2-Nitropropane	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	89.09	0.05											0.9								0.8				
Nitrosomorpholine	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	116.12		0.2											0.09						0.9					
3-Nitrotoluene / m-Nitrotoluene	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	137.14	w											0.3								0.3				
Nitrous Oxide / Dinitrogen oxide	N <sub>2</sub> O	44.01					0.03	0.5																		
Nonane	C <sub>9</sub> H <sub>20</sub>	128.26	0.007						0.4																	
Nonenal (Trans-2-nonenal)	C <sub>9</sub> H <sub>16</sub> O	140.22	0.03										0.2				0.5									
Novac 5110	C <sub>5</sub> F <sub>10</sub> O	266.04								0.003	0.004	0.007														
Novac 7300	C <sub>7</sub> H <sub>3</sub> F <sub>13</sub> O	350								0.002		0.007						0.04								
Octane	C <sub>8</sub> H <sub>18</sub>	114.23	0.007	0.2																						
1-Octanol	C <sub>8</sub> H <sub>18</sub> O	130.23	0.01											0.2		0.2										
1-Octene	C <sub>8</sub> H <sub>16</sub>	112.21	0.01					0.4												0.2						
Pentanal	C <sub>5</sub> H <sub>10</sub> O	86.13	0.02		s			0.3																		
Pentane	C <sub>5</sub> H <sub>12</sub>	72.15	0.01	0.3																						
2-Pentanone	C <sub>5</sub> H <sub>10</sub> O	86.13	0.01								0.1	0.2								0.8						
n-Pentyl acetate / Amyl acetate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.19	0.02	0.7						0.03					0.06											
Perfluoro-1,3-dimethylcyclohexane	C <sub>8</sub> F <sub>16</sub>	400.06									s						0.06			0.07						
Perfluoromethylcyclohexane	C <sub>7</sub> F <sub>14</sub>	350.05									s						0.03			0.1						
Phenol	C <sub>6</sub> H <sub>6</sub> O	94.11	0.6									0.008	0.1		0.4											
Phenylhydrazine	C <sub>8</sub> H <sub>8</sub> N <sub>2</sub>	108.14	vw								m														m	
1-Phenylpropane	C <sub>9</sub> H <sub>12</sub>	120.19	0.02						0.6																	s
Phosgene / Carbonylchloride	COCl <sub>2</sub>	98.92																			0.02	0.02				
Phosphine	PH <sub>3</sub>	34.00												0.3		0.5										
Phthalic anhydride	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	148.1												0.2						0.5						0.3
α-Pinene	C <sub>10</sub> H <sub>16</sub>	136.23	0.009											0.4									0.6			
Propadiene	C <sub>3</sub> H <sub>4</sub>	40.06	0.8																		0.1					
Propane	C <sub>3</sub> H <sub>8</sub>	44.10	0.02	0.4																						
1,2-Propanediol / Propylene glycol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	76.09	s												0.01						m					
Propanoic acid	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.08	0.1										0.03				0.3									
Propanol	C <sub>3</sub> H <sub>8</sub> O	60.10	s	0.3											0.08											
2-Propanol	C <sub>3</sub> H <sub>8</sub> O	60.10	0.02								0.09	0.07								0.2						
Propene	C <sub>3</sub> H <sub>6</sub>	42.08	0.05														0.4				0.3					
n-Propyl acetate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.13	m								s					m				m					w	
2-Propyl acetate / Isopropyl acetate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.13	m									s			s				m		m					
Propylene glycol / 1,2-Propanediol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	76.09	s												0.01							m				
Propylene glycol monomethyl ether acetate	C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>	132.16									0.01		0.02	0.03												
Propylene oxide	C <sub>3</sub> H <sub>6</sub> O	58.08	s										0.7									0.2				
Propyl nitrate	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	105.09	s														s		s					m		

Name	Brutto-formula	Molec.-weight	987 3.4 2950	986 3.6 2800	989 3.7 2750	983 4.4 2270	985 4.5 2215	984 4.7 2150	968 7.7 1291	969 8.0 1254	970 8.2 1217	971 8.5 1179	972 8.8 1139	973 9.1 1101	974 9.4 1061	936 9.8 1020	975 10.2 981	988 10.6 946	976 10.6 941	977 11.1 900	978 11.6 861	979 12.2 822	980 12.8 783	981 13.4 746	982 14.1 710	
Propyne / Methylacetylene	C <sub>3</sub> H <sub>4</sub>	40.06	0.06							0.4																
Pyridine	C <sub>5</sub> H <sub>5</sub> N	79.10	0.4													0.7									0.3	
Selenium hexafluoride	SeF <sub>6</sub>	192.95							0.4														0.01		0.2	
Sevoflurane	C <sub>4</sub> H <sub>3</sub> F <sub>7</sub> O	200.06	0.08							0.006		0.01								0.2					0.3	
Silane	SiH <sub>4</sub>	32.12																s		m						
Silicon tetrafluoride	SiF <sub>4</sub>	104.08												0.03	0.02											
Styrene	C <sub>8</sub> H <sub>8</sub>	104.15	0.1																0.3				0.2			
Sulfur dioxide	SO <sub>2</sub>	64.06									0.4	0.3														
Sulfur hexafluoride	SF <sub>6</sub>	146.06															0.009	0.006	0.004							
1,1,2,2-Tetrabromoethane	C <sub>2</sub> H <sub>2</sub> Br <sub>4</sub>	345.65	vw									m									s				m	
1,1,2,2-Tetrachloroethane	C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	167.85								0.2												0.1		0.06		
Tetrachloroethene	C <sub>2</sub> Cl <sub>4</sub>	165.83																	0.04	0.07			0.2			
Tetrachloromethane	CCl <sub>4</sub>	153.82																				0.03	0.02			
Tetraethylplumbane	C <sub>8</sub> H <sub>20</sub> Pb	323.44	s										0.2								s					
Tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O	72.11	0.01												0.09			0.5								
Tetrahydrothiophene	C <sub>4</sub> H <sub>8</sub> S	88.17	0.02									m										2				
Thionyl chloride	Cl <sub>2</sub> OS	118.97							0.02		s															
Thionyl fluoride	F <sub>2</sub> OS	86.06																					m		0.07	s
Thiophene	C <sub>4</sub> H <sub>4</sub> S	84.14									s											m				
Toluene	C <sub>7</sub> H <sub>8</sub>	92.14	0.05												0.5									0.4	0.2	
2,4-Toluenediamine	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub>	122.17	w									m											m			
2,4-Toluene diisocyanate (TDI)	C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	174.16					s															m				
o-Toluidine / o-Methylanilin	C <sub>7</sub> H <sub>9</sub> N	107.15	0.05							0.1															0.1	
Total Organic Carbon ref. Methane (TOC)			0.1																							
Total Organic Carbon ref. Propane (TOC)			0.02																							
Total Organic Carbon ref. Toluene (TOC)			0.05																							
1,2,4-Trichloro benzene	C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	181.45												s		0.4							s			
1,1,1-Trichloroethane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	133.40	0.3											0.04											0.08	
1,1,2-Trichloroethane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	133.40	0.7								0.4									0.3					0.07	
Trichloroethene	C <sub>2</sub> HCl <sub>3</sub>	131.39		0.3						0.4					4					0.07		0.08				
Trichloronitromethane / Chloropicrine	CCl <sub>3</sub> NO <sub>2</sub>	164.38	w							0.3								0.4		0.03						
1,2,3-Trichloropropane	C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub>	147.43	w								m									m					s	
Triethylamine (TEA)	C <sub>6</sub> H <sub>15</sub> N	101.19	0.02								0.1					0.1										
Trifluoromethylidid	CF <sub>3</sub> I	195.91									s			0.01											m	
Trimethylamine (TMA)	C <sub>3</sub> H <sub>9</sub> N	59.11	0.03	0.02							0.2				0.1											
1,2,4-Trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	120.19	0.2													0.5							0.3			
3,5,5-Trimethyl-2-cyclohexen-1-one / Isophorone	C <sub>9</sub> H <sub>14</sub> O	138.21	0.03	0.06						0.1			0.5								0.5					
1,3,5-Trioxane	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	90.08	w	0.09											0.08					0.09						
Undecane	C <sub>11</sub> H <sub>24</sub>	156.31	0.005	0.07																						
Vinyl acetate	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	86.09	0.4								0.007		0.03										0.1			
Vinyl chloride	C <sub>2</sub> H <sub>3</sub> Cl	62.50														0.4					0.2				0.4	
m-Xylene	C <sub>8</sub> H <sub>10</sub>	106.17	0.03	0.7											0.9								0.2	0.4		

Notification used in the chart:

  = Measured detection limit – verified by LumaSense laboratory in Denmark

Normal = Calculated detection limit

Relative strenght of absorption band:

vw = very weak

w = weak

m = medium

s = strong

vs = very strong

Calibration price group:

1 = UA0181 Automated Calibration

2 = UA0182 Advanced Calibration

3 = UA0183 Complex Calibration

# Converting concentration units

The detection limits listed on this wall chart are given in “parts per million” by volume (ppm) at 20°C and 1 atmosphere of pressure. These values can be converted into the concentration unit “mg/m<sup>3</sup>” by using equation (1) given in the box below.

For a gas at 20°C and at 1 atmosphere of pressure: (1)

$$\text{Concentration (mg/m}^3\text{)} = \frac{\text{Concentration (ppm)} \times \text{Molec. Weight (g/mol)}}{24.04 \text{ l/mol}}$$

## To Convert ppm to mg/m<sup>3</sup> (at 20°C and 1 atm.):

Reading from the chart, the detection limit at 20°C and 1 atmosphere pressure of Toluene is 0.5 ppm using the UA0974. The molecular weight of Toluene is 92.14 g/mol. Using equation (1) shown in the box above, the detection limit can be calculated in mg/m<sup>3</sup>:

$$\text{Detection Limit} = \frac{0.5 \times 92.14}{24.04} = 1.92 \text{ mg/m}^3$$

## To convert measured gas concentrations from mg/m<sup>3</sup> to ppm (at T °C and P atm.):

Equation (1) can only be used to convert concentration units of a gas measured at a pressure of 1 atmosphere and at a temperature of 20°C. If the gas is at a pressure of P atmospheres and its temperature is T Kelvin, then the conversion equation becomes:

$$\text{Concentration (ppm)} = \frac{\text{Concentration (mg/m}^3\text{)} \times \text{Molar Volume (l/mol)}}{\text{Molec. Weight (g/mol)}}$$

Where:

*Molec. Weight* = molecular weight of the substance (in g/mol). This can be found in the Detection Limit Chart.

*Molar Volume* = is the volume occupied by one mole of an ideal gas at a specified temperature and pressure. Table 3 lists the molar volume of a gas at various temperatures and 1 atmosphere of pressure. Its value at a temperature of T K and a pressure of P atmosphere can be calculated from the following equation:

*Molar Volume* =  $RT/P$ , where:

T = temperature of the gas in K,

R = Gas Constant =  $8.2054 \times 10^{-2}$  liter atm. K<sup>-1</sup> mole<sup>-1</sup>

P = pressure of the gas in atmospheres

Table 3. Molar Volume of an ideal gas at 1 atmosphere of pressure at different temperatures															
Temperature (°C)	-20	-15	-10	-5	0	5	10	15	20	25	30	35	40	45	50
Molar Volume (l/mol)	20.76	21.17	21.58	21.99	22.40	22.81	23.22	23.63	24.04	24.45	24.86	25.27	25.68	26.07	26.50

# Calculation of detection limits for different SIT settings

To calculate the detection limit at Sample Integration Times (SIT) other than 5 seconds, the following equation must be used:

$$\text{Detection limit} = \text{Detection limit in chart} \times \text{DLF}$$

The factor DLF can be read in Table 1.

Example: Reading from the chart - the detection limit for Sulphur hexafluoride (SF<sub>6</sub>) using the optical filter UA0988 is 0.006 ppm. Calculating the detection limit using SIT of 0.5 second and 50 seconds gives the following result: Detection limit SF<sub>6</sub> (SIT of 0.5) = 0.006 ppm x 3.2 = 0.019 ppm

Detection limit SF<sub>6</sub> (SIT of 50) = 0.006 ppm x 0.3 = 0.002 ppm