Advanced Energy®

# GAS DETECTION LIMITS

Highly Accurate, Reliable, and Stable Gas Monitoring

## About Advanced Energy

Advanced Energy enables customer innovation by delivering highly proprietary products with differentiated performance & value. We design and manufacture highly engineered, precision power conversion, measurement, and control solutions for mission-critical applications and processes.

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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 Advanced Energy using various optical filters

Since most gases have characteristic infrared absorption spectra, infrared spectroscopy is an excellent monitoring tool. Advanced Energy 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.

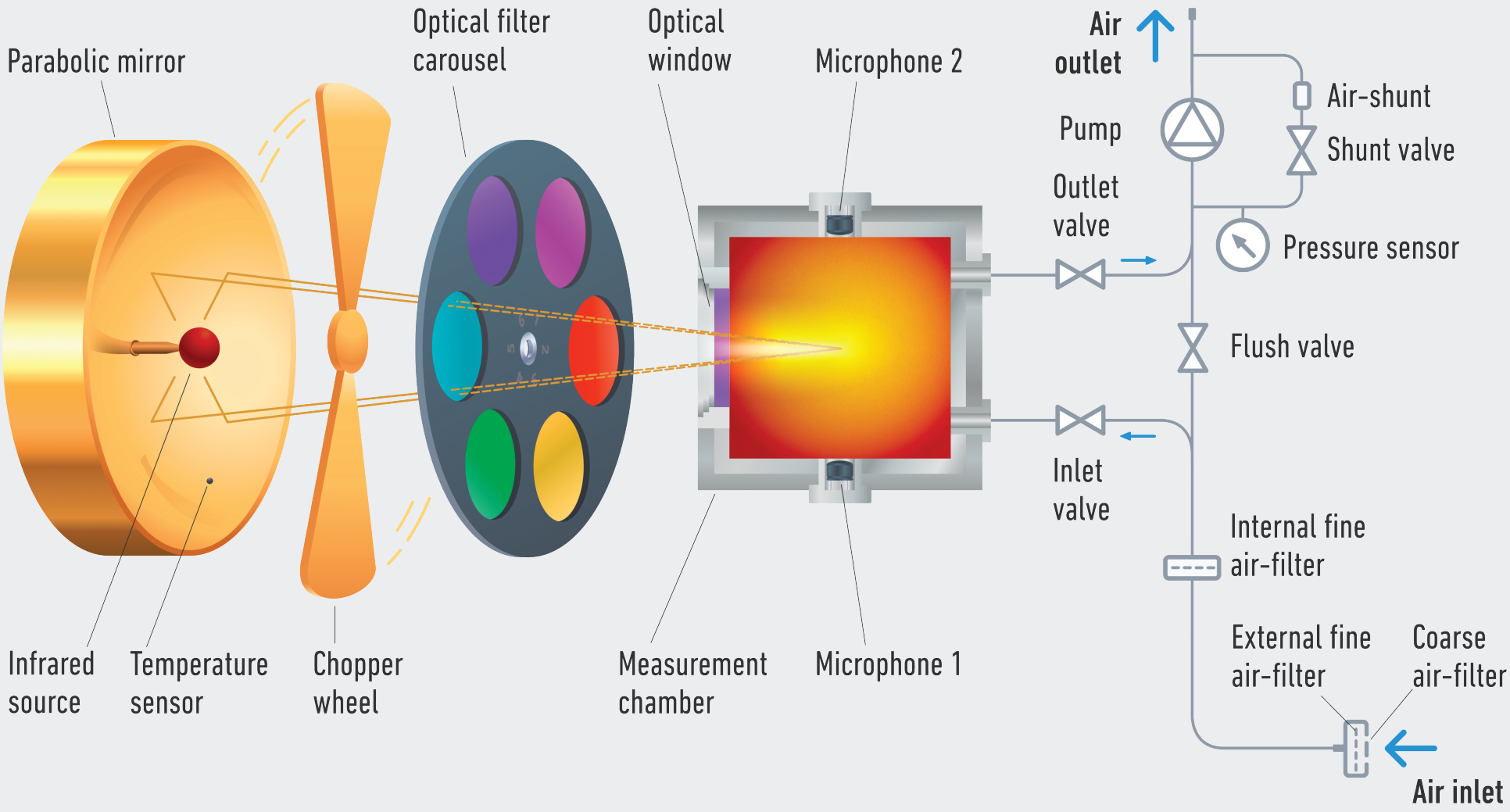
Included with the 1512 and the 1314i is user software. The software displays measurement data in a table or a graphical window and it uses a SQL Server 2014 database giving online access to measurement data from Microsoft® Excel.

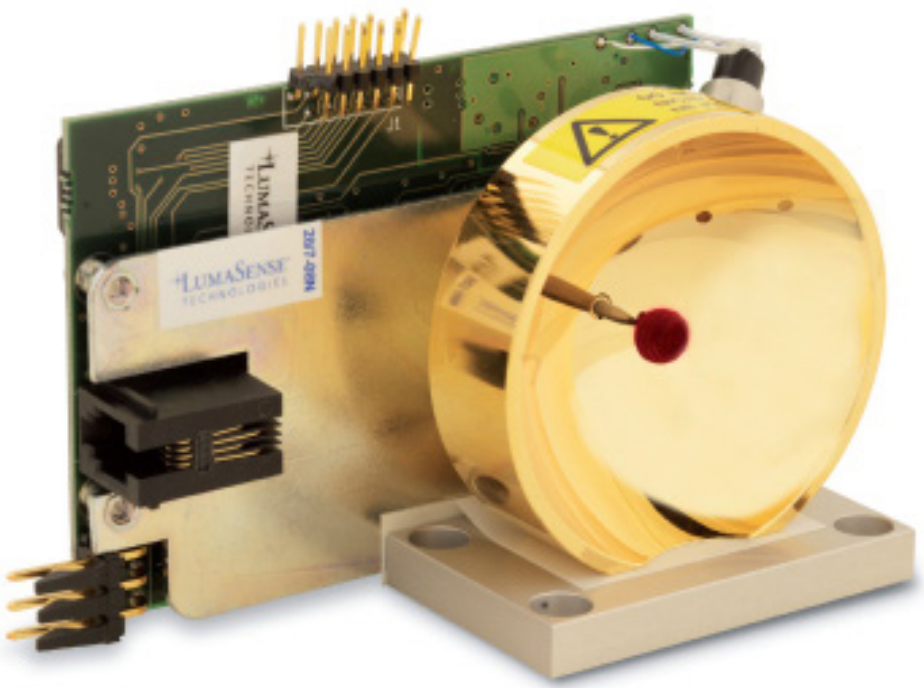

PHOTOACOUSTIC GAS MONITOR – INNOVA 1512


PHOTOACOUSTIC GAS MONITOR – INNOVA 1314i

# Photoacoustic Spectroscopy (PAS)

**PAS system used in the Innova instruments**



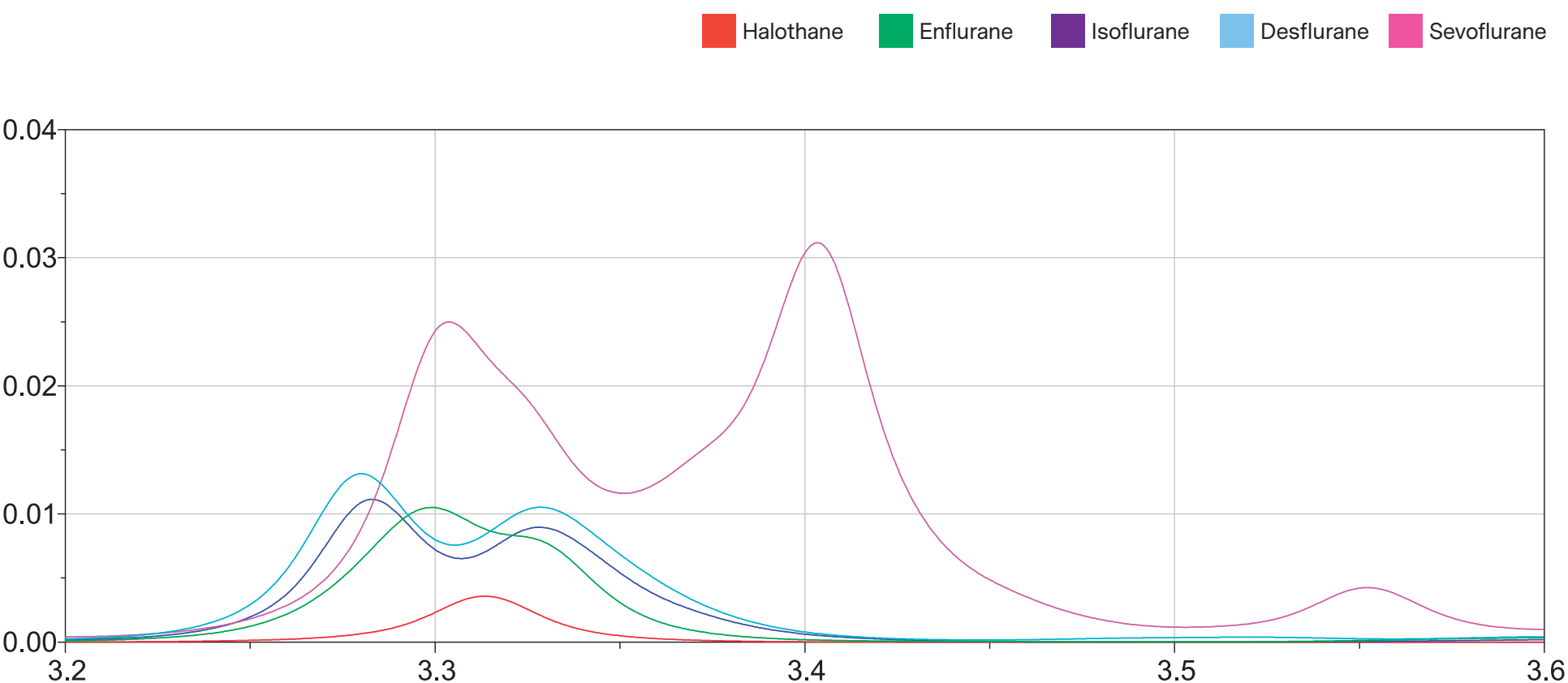



UNIT OF IR-SOURCE WITH ELLIPSOID MIRROR


UNIT OF PAS MEASUREMENT CELL

## Infrared spectra

The → C – H fundamenttal stretching vibration frequencies are always in the region from 3.2 to 3.6 µm. 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 $cm^{-1}$) plus the region between 2000 and 3000 $cm^{-1}$ (see Fig. 1 and Table 1). The "gap" in the infrared spectrum between 1350 $cm^{-1}$ and 2000 $cm^{-1}$ 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.

### 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.

Note: All optical filters listed comply with MIL-SC-48497A requirements.

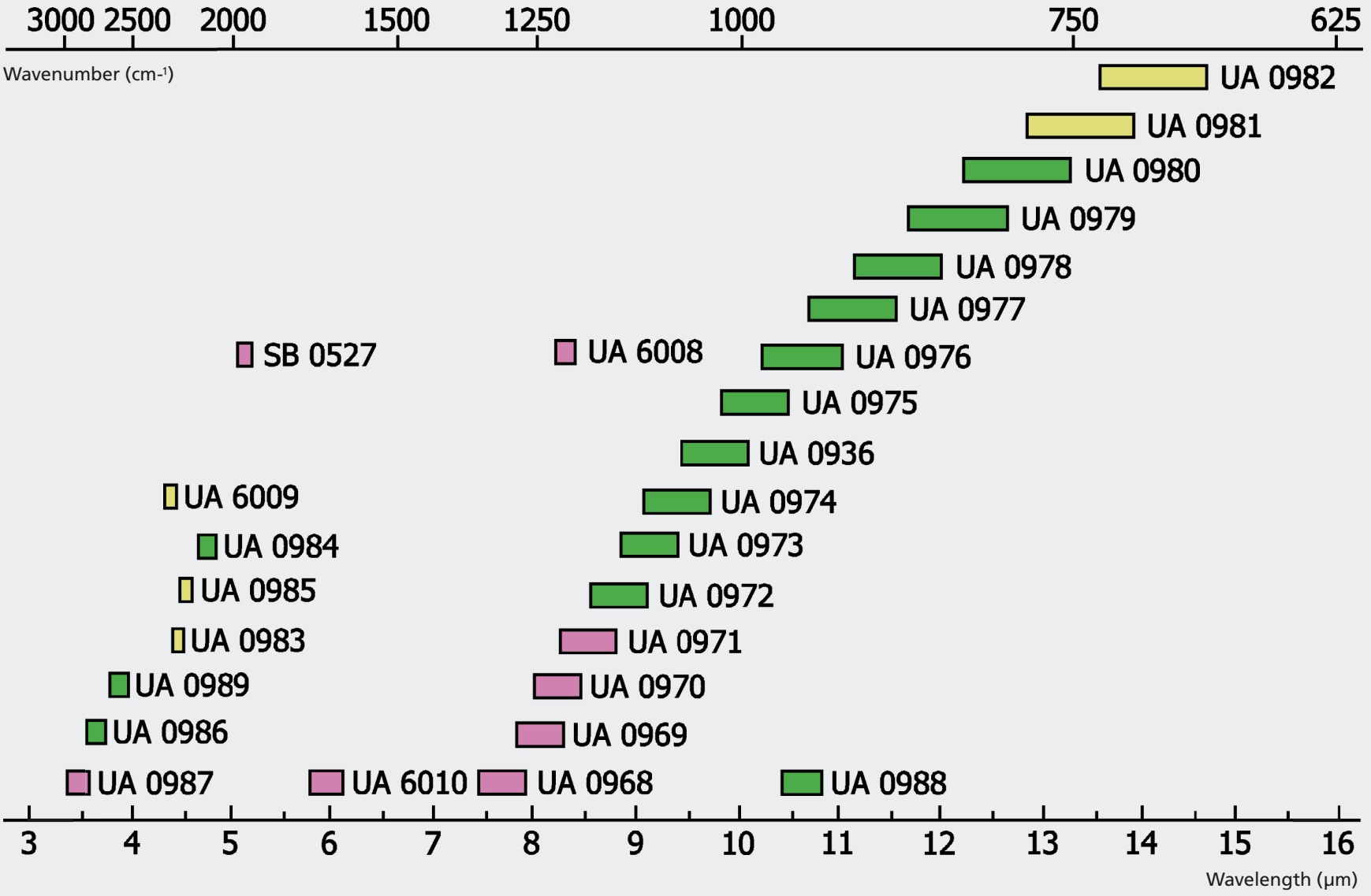
**Table 1. Filter specifications**

| Optical Filter Number | Filter Centre µm | Filter Centre $cm^{-1}$ | 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.

**Table 2. Detection Limit Factor as a function of Sample Integration Time**

| 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 x 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 Advanced Energy representative is contacted for help in choosing the optimum filter configuration.

Notification used in the chart:

= Measured detection limit verified by Advanced Energy laboratory

Normal = Calculated detection limit

Relative strenght of absorption band:

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

| Detection limits in part per million at 20°C, 1 atmosphere pressure and SIT=5 sec. | | | Optical filter number<br>Centre wavelength (in micrometer)<br>Centre wavenumber (in $cm^{-1}$) | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Name | Brutto-formula | Molec.-weight | 987<br>3.4<br>2950 | 986<br>3.6<br>2800 | 989<br>3.7<br>2750 | 983<br>4.4<br>2270 | 985<br>4.5<br>2215 | 984<br>4.7<br>2150 | 968<br>7.7<br>1291 | 969<br>8.0<br>1254 | 970<br>8.2<br>1217 | 971<br>8.5<br>1179 | 972<br>8.8<br>1139 | 973<br>9.1<br>1101 | 974<br>9.4<br>1061 | 936<br>9.8<br>1020 | 975<br>10.2<br>981 | 988<br>10.6<br>946 | 976<br>10.6<br>941 | 977<br>11.1<br>900 | 978<br>11.6<br>861 | 979<br>12.2<br>822 | 980<br>12.8<br>783 | 981<br>13.4<br>746 | 982<br>14.1<br>710 |
| Acetaldehyde | $C_2H_4O$ | 44.05 | 0.1 | 0.08 | 0.2 | | | | | | | | 0.2 | 0.2 | | | | | | | | | | | |
| Acetic acid | $C_2H_4O_2$ | 60.05 | | | | | | | | | 0.04 | 0.03 | | | | | | | | | | | | | |
| Acetic anhydride | $C_4H_6O_3$ | 102.09 | | | | | | | | 0.04 | | | | | 0.05 | | | | | 0.1 | | | | | |
| Acetone | $C_3H_6O$ | 58.08 | 0.1 | | | | | | | 0.07 | 0.06 | | | | | | | | | | | | | | |
| Acetonitrile | $C_2H_3N$ | 41.05 | w | | w | | | | | | | | | | 2.5 | w | | | | w | | | | | |
| Acetylene | $C_2H_2$ | 26.04 | | | | | | | | 1 | | | | | | | | | | | | | 0.3 | 0.3 | 0.3 |
| Acrolein | $C_3H_4O$ | 56.06 | 0.1 | 0.1 | m | | | | | | | | 0.2 | | | 0.09 | | | 0.1 | | | | | | |
| Acrylonitrile | $C_3H_3N$ | 53.06 | | | | | | | | | | | | | | 0.3 | 0.2 | | 0.2 | | | | | | |
| Allyl chloride | $C_3H_5Cl$ | 76.52 | 0.2 | | | | | | | 0.2 | | | | | | | | | 0.2 | | | | | 0.4 | |
| Ammonia | $NH_3$ | 17.03 | | | | | | | | | | | | 0.2 | | | 0.2 | | 0.2 | | | | | | |
| Aniline | $C_6H_7N$ | 93.13 | 0.3 | | | | | | | 0.09 | | | | | 0.2 | | | | | | | | | 0.2 | |
| Arsine | $AsH_3$ | 77.95 | | | | | 0.05 | 0.03 | | | | | | | | | 0.4 | | 0.4 | | | | | | |
| Benzaldehyde | $C_7H_6O$ | 106.12 | | 0.07 | | | | | | | | 0.09 | | | | | | | | | | | | 0.3 | |
| Benzene | $C_6H_6$ | 78.11 | 0.1 | | | | | | | | | | | | 0.9 | 0.8 | 21 | | | | | | | | 0.3 |
| Benzyl chloride / α-Chlorotoluene | $C_7H_7Cl$ | 126.58 | 0.1 | | | | | | | 0.1 | | | | | | | | | | | | | | 0.3 | 0.1 |
| Biphenyl | $C_{12}H_{10}$ | 154.21 | m | | | | | | | | | | | | | | | | | w | | | | | |
| Boron trifluoride | $BF_3$ | 67.81 | | | | | | | | | | | | | | 0.2 | | | | | | | | 0.07 | |
| Bromoform / Tribromomethane | $CHBr_3$ | 252.73 | vw | | | | | | | | | 0.1 | 0.06 | 12 | | | | | | | | | | | 1 |
| Bromomethane | $CH_3Br$ | 94.94 | 0.2 | | | | | | 0.5 | | | | | | | | | | | | | | | | |
| 1,3-Butadiene | $C_4H_6$ | 54.09 | 0.2 | | | | | | | | | | | | | 0.2 | | | 0.1 | 0.2 | | | | | |
| Butane | $C_4H_{10}$ | 58.12 | 0.01 | 0.5 | | | | | | | | | | | | | | | | | | | | | |
| Butane-2,3-dione | $C_4H_6O_2$ | 86.09 | | | | | | | | | | | 0.06 | 0.06 | | | | | | | | | | | |
| Butanethiol / Butyl mercaptan | $C_4H_{10}S$ | 90.19 | s | | | | | | | s | | | | | | | | | | | | m | | | |
| 1-Butanol | $C_4H_{10}O$ | 74.12 | 0.01 | | | | | | | 0.2 | | | | | 0.08 | | | | 0.5 | | | | | | |
| 2-Butanol | $C_4H_{10}O$ | 74.12 | s | | | | | | | | | | m | | | m | | | | m | | | | | |
| tert-Butanol / tert-Butyl alcohol | $C_4H_{10}O$ | 74.12 | 0.03 | | | | | | | | | | 0.08 | | | | | | | 0.2 | | | | | |
| 2-Butanone / Methyl ethyl ketone(MEK) | $C_4H_8O$ | 72.11 | 0.04 | 1 | | | | | | | 0.2 | 0.07 | | | | | | | 0.5 | | | | | | |
| 2-Butenal / Crotonaldehyde | $C_4H_6O$ | 70.09 | m | m | s | | | | | | | | s | 0.2 | | | s | | | | | | | | |
| 2-Butoxyethanol | $C_6H_{14}O_2$ | 118.17 | 0.01 | | | | | | | | | 0.05 | 0.04 | | | | | | | | 0.4 | | | | |
| n-Butyl acetate | $C_6H_{12}O_2$ | 116.16 | 0.02 | | | | | | | 0.01 | | | | 0.08 | 0.05 | | | | | | | | | | |
| sec-Butyl acetate | $C_6H_{12}O_2$ | 116.16 | s | | | | | | | s | | | | s | | | | m | | | | | | | |
| tert-Butyl acetate | $C_6H_{12}O_2$ | 116.16 | s | | | | | | | s | | s | | | | | | | | | | | | | |
| Butyl acrylate | $C_7H_{12}O_2$ | 128.17 | 0.02 | 0.02 | | | | | | | 0.02 | | | 0.09 | | | | | | | | | | | |
| tert-Butyl alcohol / tert-Butanol | $C_4H_{10}O$ | 74.12 | 0.03 | | | | | | | | | | 0.08 | | | | | | | 0.2 | | | | | |
| Butyraldehyde | $C_4H_8O$ | 72.11 | s | s | | | | | | | | | | | | | | | | | | | | 1 | |
| Butyric acid | $C_4H_8O_2$ | 88.11 | 0.04 | | | | | | | | | | 0.04 | 0.06 | | | | | | | | | | | |
| Carbon dioxide | $CO_2$ | 44.01 | | | | 5 | 70 | | | | | | | | | | | | | | | | | 13 | 1.5 |
| Carbon disulfide | $CS_2$ | 76.14 | | | | | 1 | 0.6 | | | | | | | | | | | | | | | | | |
| Carbon monoxide | CO | 28.01 | | | | | 0.5 | 0.2 | | | | | | | | | | | | | | | | | |
| Carbonyl chloride / Phosgene | $COCl_2$ | 98.92 | | | | | | | | | | | | | | | | | | | 0.02 | 0.02 | | | |
| Carbonyl sulfide | COS | 60.08 | 0.3 | | | | | 1 | | | | | | | | | | | | | 0.6 | | | | |
| Chlorobenzene | $C_6H_5Cl$ | 112.56 | | | | | | | | | | | | 0.09 | 0.2 | | | | | | | | | | 0.2 |
| 2-Chloroethyl ether | $C_4H_8Cl_2O$ | 143.01 | 0.03 | 0.4 | | | | | | 0.4 | | | 0.02 | 0.02 | | | | | | | | | | | |
| Chloroform | $CHCl_3$ | 119.38 | | | | | | | | | 0.09 | | | | | | | | | | | 0.3 | 0.04 | | |
| Chloromethane | $CH_3Cl$ | 50.49 | 0.2 | | | | | | | | | | | | | 2 | | | | | | | | 0.6 | |
| 1-Chloro-1-nitropropane | $C_3H_6ClNO_2$ | 123.54 | m | | | | | | | m | | | | | | | | m | | | m | | | | |
| α-Chlorotoluene / Benzyl chloride | $C_7H_7Cl$ | 126.58 | 0.1 | | | | | | | 0.1 | | | | | | | | | | | | | | 0.3 | 0.1 |
| m-Cresol / 3-Methylphenol | $C_7H_8O$ | 108.14 | 0.07 | | | | | | | | | 0.05 | | | | | | | 0.3 | | | | | 0.3 | |
| Crotonaldehyde / 2-Butenal | $C_4H_6O$ | 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 | $C_9H_{12}$ | 120.19 | m | | | | | | | | | | | m | | 0.7 | | | | | | | m | | |
| Cyanogen / Dicyan | $C_2N_2$ | 52.03 | | | | | 1.1 | 0.6 | | | | | | | | | | | | | | | | | |
| Cyanogen bromide | BrCN | 105.92 | | | | | 0.1 | | | | | | | | | | | | | | | | | | |
| Cyanogen chloride | CNCl | 61.47 | | | | | 0.3 | 0.4 | | | | | | | | | | | | | | | | | |
| Cyclohexane | $C_6H_{12}$ | 84.16 | 0.008 | 0.2 | | | | | | 0.7 | | | | | | | | | | | | | | | |
| Cyclohexanone | $C_6H_{10}O$ | 98.14 | s | | | | | | | | 0.2 | | | | | | | | | m | | | | | |
| Cyclohexene | $C_6H_{10}$ | 82.14 | 0.02 | | | | | | | | | | | | | | | | | 0.9 | | | | | |
| Cyclopentane | $C_5H_{10}$ | 70.1 | vs | 0.7 | | | | | | | | | | | | | | m | | | | | | | |
| n-Decane | $C_{10}H_{22}$ | 142.28 | 0.007 | | | | | | 0.3 | | | | | | | | | | | | | | | | |
| 1-Decene | $C_{10}H_{20}$ | 140.27 | 0.009 | | | | | | 0.3 | | | | | | | | | | 0.3 | | | | | | |
| Desflurane | $C_3H_2F_6O$ | 168.04 | | | | | | | | | 0.005 | | 0.008 | | | | | | | | | | | | m |
| Deuterium oxide | $D_2O$ | 20.03 | | 0.3 | | | | | | s | | | | s | | | | | | | | | | | |
| Diamine / Hydrazine | $N_2H_4$ | 32.05 | | | | | | | | | | | | | 0.6 | 0.6 | | | | | 0.6 | | | | |
| Diaminoethane | $C_2H_8N_2$ | 60.10 | 0.04 | | | | | | | | | | | 0.7 | | | | | | | | | 0.1 | | |
| Diborane | $B_2H_6$ | 27.67 | | | | | | | | | | 0.1 | 0.1 | | | | | | | | | | | | |
| o-Dichlorobenzene / 1,2-Dichlorobenzene | $C_6H_4Cl_2$ | 147.00 | 4 | | | | | | | | | | | | 0.3 | | | | | | | | | 0.1 | |
| m-Dichlorobenzene / 1,3-Dichlorobenzene | $C_6H_4Cl_2$ | 147.00 | 2 | | | | | | | | | | | 0.1 | | | | | | | | | 0.1 | 0.15 | |
| p-Dichlorobenzene / 1,4-Dichlorobenzene | $C_6H_4Cl_2$ | 147.00 | | | | | | | | | | | | 0.05 | 0.2 | | | | | | | 0.2 | | | |
| 1,1-Dichloroethane | $C_2H_4Cl_2$ | 98.96 | 0.2 | | | | | | | | 0.2 | | | | 0.1 | | | | | | | | | | 0.09 |
| 1,2-Dichloroethane | $C_2H_4Cl_2$ | 98.96 | 0.2 | | | | | | | 0.1 | | | | | | | | | | | | | | 0.3 | |
| 1,1-Dichloroethene | $C_2H_2Cl_2$ | 96.94 | | | | | | | | | | | | vs | | | | | | | | 0.09 | | m | |
| 1,2-Dichloroethene (cis) | $C_2H_2Cl_2$ | 96.94 | | | | | | | 0.2 | | | | | | | | | | | | 0.09 | 0.2 | | | s |
| 1,2-Dichloroethene (trans) | $C_2H_2Cl_2$ | 96.94 | | | | | | | | | | 0.2 | | | | | | | | | 0.07 | 0.05 | | | |
| Dichloromethane | $CH_2Cl_2$ | 84.93 | 0.6 | | | | | | | | 0.5 | | | | | | | | | | | | 0.1 | 0.08 | |
| 1,1-Dichloro-1-nitroethane | $C_2H_3Cl_2NO_2$ | 143.96 | | | | | | | | | | | | | m | | | | | | m | | | | m |
| 1,2-Dichloropropane | $C_3H_6Cl_2$ | 112.99 | 0.08 | | | | | | | | | 0.3 | | | | 0.3 | | | | | | | | 0.5 | |
| Diethylamine | $C_4H_{11}N$ | 73.14 | 0.02 | | | | | | | | | | 0.1 | | | | | | | | | | | 0.4 | |
| 2-(Diethylamino)-ethanol | $C_6H_{15}NO$ | 117.19 | s | | | | | | | | | m | | | 0.4 | | | | | | | | | | |
| Diethylen glycol dimethyl ether | $C_6H_{14}O_3$ | 134.17 | 0.01 | | | | | | | | | | 0.02 | 0.02 | | | | | | | | | | | |
| Diethylen glycol butyl ether | $C_8H_{18}O_3$ | 162.23 | s | m | | | | | | | | | | s | s | | | | | m | | | | | |
| Diethylentriamin | $C_4H_{13}N_3$ | 103.17 | s | | 0.4 | | | | | | | 0.4 | | | 0.3 | | | | | | | 0.3 | | | |
| Diethyl ether | $C_4H_{10}O$ | 74.12 | 0.02 | | | | | | | | | | 0.02 | 0.08 | | | | | | | | | | | |
| Diethyl ketone (DEK) / 3-Pentanone | $C_5H_{10}O$ | 86.13 | 0.01 | | | | | | | | | | 0.1 | | | | | | 0.2 | | | | | | |
| N,N-Dimethyl acetamide | $C_4H_9NO$ | 87.12 | m | | | | | | | | m | | | | | 0.3 | 0.2 | | | | | | | | |
| Dimethylamine (DMA) | $C_2H_7N$ | 45.08 | 0.02 | 0.04 | | | | | | | | | 0.1 | | | | | | | | | | 0.3 | | |
| 2-(Dimethylamino)-ethanol | $C_4H_{11}NO$ | 89.14 | s | | | | | | | | | | | vs | | | | | | | m | | | | |
| N,N-Dimethylanilin | $C_8H_{11}N$ | 121.18 | m | | | | | | | | | m | | | | m | | | | | | | | | m |
| Dimethyl disulfide | $C_2H_6S_2$ | 94.20 | s | | | | | | s | | | | | | | | | 0.6 | | | | | | | |
| Dimethyl ester sulfuric acid (DMS) | $C_2H_6O_4S$ | 126.13 | 0.07 | | | | | | | | | | | | | 0.02 | 0.06 | | | | | 0.05 | | | |
| Dimethylether | $C_2H_6O$ | 46.07 | s | | | | | | | | | | 0.07 | | 0.2 | | | | | | | | | | |
| Dimethylethylamine | $C_4H_{11}N$ | 73.14 | s | | | | | | | | 0.2 | | | 0.2 | | | | | | | | | 0.8 | | |
| Dimethylformamide (DMF) | $C_3H_7NO$ | 73.09 | 0.1 | | | | | | | | 0.3 | | | 0.06 | 0.07 | | 3 | | | | | | | 0.9 | |
| 2,6-Dimethyl-4-heptanone | $C_9H_{18}O$ | 142.24 | 0.008 | | | | | | | 0.5 | | | | 0.3 | | | | | | | | | | | |
| 1,1-Dimethylhydrazine | $C_2H_8N_2$ | 60.10 | s | | | | | | | | | | | | s | | | s | | | | s | | | |
| Dimethylnitrosamine | $C_2H_6N_2O$ | 74.08 | 0.04 | | | | | | | 0.06 | | | | | | 0.03 | | | | | | | | | |
| Dimethyl sulfoxide | $C_2H_6OS$ | 78.13 | 0.3 | | | | | | | | | | | 0.07 | | 0.6 | | | | | | | | | |
| Dimethyl sulfate | $C_2H_6O_4S$ | 126.13 | m | | | | | | | | | s | | | | vs | | | | | | 0.06 | | | |
| Dimethyl sulfide | $C_2H_6S$ | 62.13 | s | 0.4 | | | | | | | | | | | 0.7 | 0.6 | | | | | | | | | |
| Dimethyl sulfite | $C_2H_6O_3S$ | 110.13 | m | | | | | | | | s | | | | | | s | | | | | | | m | |
| Dinitrogen difluoride | $N_2F_2$ | 66.01 | | | | | | | | | | | | | | | 0.02 | 0.2 | | | | | | | |
| Dinitrogen oxide / Nitrous Oxide | $N_2O$ | 44.01 | | | | | 0.03 | 0.5 | | | | | | | | | | | | | | | | | |
| 1,4-Dioxane / 1,4-Diethylene oxide | $C_4H_8O_2$ | 88.11 | 0.02 | | | | | | | | | | 0.02 | | | | | | | 0.07 | | | | | |

| Name | Brutto-formula | Molec.-weight | 987<br>3.4<br>2950 | 986<br>3.6<br>2800 | 989<br>3.7<br>2750 | 983<br>4.4<br>2270 | 985<br>4.5<br>2215 | 984<br>4.7<br>2150 | 968<br>7.7<br>1291 | 969<br>8.0<br>1254 | 970<br>8.2<br>1217 | 971<br>8.5<br>1179 | 972<br>8.8<br>1139 | 973<br>9.1<br>1101 | 974<br>9.4<br>1061 | 936<br>9.8<br>1020 | 975<br>10.2<br>981 | 988<br>10.6<br>946 | 976<br>10.6<br>941 | 977<br>11.1<br>900 | 978<br>11.6<br>861 | 979<br>12.2<br>822 | 980<br>12.8<br>783 | 981<br>13.4<br>746 | 982<br>14.1<br>710 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Diphenyl ether | $C_{12}H_{10}O$ | 170.21 | m/w | | | | | | | s | s | | | | | | | | | s | | | | | |
| Dipropylnitrosamine | $C_6H_{14}N_2O$ | 130.19 | 0.03 | | | | | | | | | 0.1 | | | 0.05 | | | | | | | | | | |
| Enflurane | $C_3H_2ClF_5O$ | 184.49 | 0.1 | | | | | | | | | 0.007 | 0.005 | | | | | | | | | 0.08 | | | |
| Epichlorohydrin | $C_3H_5ClO$ | 92.52 | m | | | | | | | | | | 0.9 | | | | | | | | 0.2 | | | | |
| Ethane | $C_2H_6$ | 30.07 | 0.02 | | | | | | | | | | | | | | | | | | | 1 | | | |
| Ethanethiol / Ethyl mercaptan | $C_2H_6S$ | 62.13 | s | | | | | | | | | | | | | | 1 | | 2 | | | | | | |
| Ethanol | $C_2H_6O$ | 46.07 | 0.03 | | | | | | | | | | 0.2 | | 0.08 | 0.08 | | | | | | | | | |
| Ethanolamine | $C_2H_7NO$ | 61.08 | 0.09 | | | | | | | | | | | | 0.1 | | | | | | | 0.7 | | | |
| Ethene | $C_2H_4$ | 28.05 | 0.3 | | | | | | | | | | | | | | 0.2 | | | 0.4 | | | | | |
| 2-Ethoxyethanol / Cellosolve | $C_4H_{10}O_2$ | 90.12 | s | | | | | | | | | | 0.02 | | s | | | | m | | | | | | |
| 2-Ethoxy ethylacetate | $C_6H_{12}O_3$ | 132.16 | 0.02 | | | | | | 0.02 | | 0.01 | | | | | | | | 0.3 | | | | | | |
| Ethyl acetate | $C_4H_8O_2$ | 88.11 | 0.03 | | | | | | | 0.01 | | | | | 0.05 | | | | | | 0.8 | | | | |
| Ethyl acrylate | $C_5H_8O_2$ | 100.12 | 0.04 | | | | | | | | | 0.02 | | | 0.06 | | | | 0.2 | | | | | | |
| Ethylamine | $C_2H_7N$ | 45.08 | | | | | | | | | | | | 0.2 | | | | | | | | 0.07 | 0.09 | | |
| Ethyl benzene | $C_8H_{10}$ | 106.17 | 0.01 | | | | | | | | | | | | 0.5 | | | | | | | | | 0.4 | 0.09 |
| Ethylene glycol / Ethanediol | $C_2H_6O_2$ | 62.07 | m | | | | | | | | | | | 0.08 | 0.05 | | | | | | m | | | | |
| Ethylene oxide | $C_2H_4O$ | 44.05 | 0.08 | | | | | | | 0.3 | | | | | | | | | | 0.2 | 0.1 | | | | |
| Ethyl formate | $C_3H_6O_2$ | 74.08 | 0.03 | | | | | | | | | 0.03 | | | | 0.4 | | | | | | | | | |
| 2-Ethyl-1-Hexanol | $C_8H_{18}O$ | 130.23 | 0.008 | | | | | | | | | | | | 0.08 | | 0.3 | | | | | | | | |
| Ethylhexyl acrylate | $C_{11}H_{20}O_2$ | 184.28 | s | | | | | | | | | 0.03 | | | | m | | | 0.4 | | | | | | |
| 5-Ethyl-2-methylpyridine | $C_8H_{11}N$ | 121.18 | s | | | | | | | | | | | | m | | | | | | | 0.6 | | | |
| Fluorobenzene | $C_6H_5F$ | 96.10 | 7 | | | | | | | | 0.03 | | | | | | | | | | | | | 0.2 | |
| Formaldehyde | $CH_2O$ | 30.03 | 0.1 | 0.04 | 0.1 | | | | | | | | | | | | | | | | | | | | |
| Formic acid | $CH_2O_2$ | 46.03 | 0.01 | | | | | | | | 0.2 | | 0.04 | 0.02 | | | | | | | | | | | |
| Freon 11 / Trichlorofluoromethane | $CCl_3F$ | 137.37 | | | | | | | | | | | | 0.04 | 0.04 | | | | | | 0.02 | | | | |
| Freon 12 / Dichlorodifluoromethane | $CCl_2F_2$ | 120.91 | | | | | | | | | | 0.02 | 0.02 | | | | | | | 0.03 | | | | | |
| Freon 12B2 / Dibromodifluoromethane | $CBr_2F_2$ | 209.82 | | | | | | | | | | | | 0.08 | 0.1 | | | | | | | 0.1 | | | |
| Freon 13 / Chlorotrifluoromethane | $CClF_3$ | 104.46 | | | | | | | | | 0.02 | 0.04 | | 0.05 | | | | | | | | | | | |
| Freon 14 / Tetrafluoromethane | $CF_4$ | 88.00 | | | | | | | | 0.004 | 0.08 | | | | | | | | | | | | | | |
| Freon 21 / Dichlorofluoromethane | $CHCl_2F$ | 102.92 | vw | | | | | | | | | | | 0.01 | | | | | | | | 0.02 | | | |
| Freon 22 / Chlorodifluoromethane | $CHClF_2$ | 86.47 | 0.3 | | | | | | | | | | 0.02 | 0.01 | | | | | | | | | 0.2 | | |
| Freon 23 / Trifluoromethane | $CHF_3$ | 70.01 | m | | | | | | | | | | 0.007 | | | | | | | | | | | | |
| Freon 32 / Difluoromethane | $CH_2F_2$ | 52.02 | | | | | | | | | | | 0.04 | 0.01 | 0.03 | | | | | | | | | | |
| Freon 112 / 1,1,2,2-Tetrachloro-1,2-difluoroethane | $C_2Cl_4F_2$ | 203.83 | | | | | | | | | | | s | s | | s | | | | s | | | | | |
| Freon 113 / 1,1,2-Trichloro-1,2,2-trifluoroethane | $C_2Cl_3F_3$ | 187.38 | 0.4 | | | | | | | | 0.02 | 0.02 | | | 0.03 | | | | | | | 0.04 | | | |
| Freon 114 / 1,2-Dichlorotetrafluoroethane | $C_2Cl_2F_4$ | 170.92 | | | | | | | | | 0.01 | | 0.01 | | | | | | | | 0.02 | | | | |
| Freon 115 / Chloropentafluoroethane | $C_2ClF_5$ | 154.47 | | | | | | | | | | 0.001 | | 0.003 | | | 0.001 | | | | | | | | |
| Freon 116 / Hexafluoroethane | $C_2F_6$ | 138.01 | | | | | | | | 0.01 | | | | 0.02 | | | | | | | | | | | |
| Freon 134a / Tetrafluoroethane | $C_2H_2F_4$ | 102.03 | 0.05 | | | | | | | | | 0.01 | 0.04 | | | | | | 0.2 | | | | | | |
| Freon 141b/1,1-Dichloro-1-fluoroethane | $C_2H_3Cl_2F$ | 116.95 | | | | | | | | | | | | | | | 0.6 | | | | | | 0.1 | | |
| Freon 152 / 1,2-Difluoroethane | $C_2H_4F_2$ | 66.05 | 0.08 | | | | | | | | | | 0.002 | | | | | | 0.09 | | | | | | |
| Freon152a / 1,1-Difluoroethane | $C_2H_4F_2$ | 66.05 | vw | | | | | | | | | 0.05 | 0.01 | | | | | | | | | | | | |
| Freon 160 / Chloroethane | $C_2H_5Cl$ | 64.51 | 0.06 | | | | | | | 0.2 | | | | | | | 0.4 | | | | | | | | |
| Freon 227 / 1,1,1,2,3,3,3-Heptafluoropropane | $C_3HF_7$ | 170.03 | | | | | | | | 0.005 | 0.007 | | 0.01 | | | | | | | | | | | | |
| Freon 1113 / Chlorotrifluoroethene | $C_2ClF_3$ | 116.47 | | | | | | | | 0.07 | | | | | 0.04 | | | | | | | | | | |
| Freon 404a | | | | | | | | | | | | | | 0.2 | | | 0.1 | | | | | | | | |
| Furfural | $C_5H_4O_2$ | 96.08 | | 0.2 | | | | | | | | | | | | 0.1 | | | | | | | 0.2 | | |
| Furfuryl alcohol | $C_5H_6O_2$ | 98.10 | m | | | | | | | | | | s | | | | 0.1 | | | | | | | s | |
| Glutaraldehyde | $C_5H_8O_2$ | 100.12 | | 0.2 | 0.06 | | | | | | | | | | | | | | | | | 0.7 | | | |
| Halothane | $C_2HBrClF_3$ | 197.38 | 0.9 | | | | | | | | | 0.02 | 0.02 | | | | | | | | | 0.09 | | | |
| 1,1,1,2,3,3,3-Heptafluoropropane | $C_3HF_7$ | 170.03 | | | | | | | | 0.005 | 0.007 | | 0.02 | | | | | | | | | | | | |
| n-Heptane | $C_7H_{16}$ | 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 | $C_7H_{14}O$ | 114.19 | 0.01 | 0.2 | | | | | | | | 0.3 | | | | | | | | | | | | | |
| 3-Heptanone | $C_7H_{14}O$ | 114.19 | m | | | | | | | | | | | m | | m | | | | | | | | | |
| Hexachloroethane | $C_2Cl_6$ | 236.74 | | | | | | | | | | | | | | | | | | | | | s | | |
| Hexafluorobenzene | $C_6F_6$ | 186.05 | | | | | | | | | | | | | | 0.01 | 0.02 | | | | | | | | |
| Hexanal | $C_6H_{12}O$ | 100.16 | 0.02 | m | s | | | | 0.2 | | | | | | | | | | | | | | | | |
| n-Hexane | $C_6H_{14}$ | 86.18 | 0.009 | 0.1 | | | | | | | 0.2 | | | | | | | | | | | | | | |
| Hexanoic acid | $C_6H_{12}O_2$ | 116.16 | s | | | | | | | | | m | | | | | | m | | | | | | | |
| Hexanol | $C_6H_{14}O$ | 102.17 | 0.02 | | | | | | | | | | | | s | s | | | | | | | | | |
| 1-Hexene | $C_6H_{12}$ | 84.16 | 0.01 | | | | | | | | | | | | | | | | | 0.2 | | | | | |
| HFO-1233zd / 1-Chloro-3,3,3-trifluoropropene | $C_3H_2ClF_3$ | 130.49 | | | | | | | | | | 0.01 | 0.009 | | | | | | | | 0.07 | | | | |
| HFO 1234yf / 2,3,3,3-Tetrafluoropropene | $C_3H_2F_4$ | 114.04 | | | | | | | | | vs | 0.01 | | 0.3 | | | | | 0.2 | | | | | | |
| HFO 1234ze / trans-1,3,3,3-Tetrafluoroprop-1-ene | $C_3H_2F_4$ | 114.04 | | | | | | | | | | | 0.05 | 0.05 | | | | | 0.5 | | | | | | |
| Hydrazine / Diamine | $N_2H_4$ | 32.05 | | | | | | | | | | | | | 0.6 | 0.6 | | | | | 0.6 | | | | |
| Hydrogenchloride | HCl | 36.46 | | 0.4 | | | | | | | | | | | | | | | | | | | | | |
| Hydrogencyanide | HCN | 27.03 | | | | | | | | | | | | | | | | | | | | | | 0.5 | 0.2 |
| Hydrogensulfide | $H_2S$ | 34.08 | | | | | | | | 14 | 22 | | | | | | | | | | | | | | |
| 4-Hydroxy-4-methyl-2-pentanone | $C_6H_{12}O_2$ | 116.16 | s | | | | | | | | | | m | | | | | | m | | | | | | |
| Isobutyl acetate / 2-Methyl-1-propyl acetate | $C_6H_{12}O_2$ | 116.16 | s | | | | | | | | s | | | | | s | | | | | | | | | |
| Isobutyl alcohol / 2-Methyl-1-propanol | $C_4H_{10}O$ | 74.12 | s | m | | | | | | | | | | | s | | | | m | | | | | | |
| Isoflurane | $C_3H_2ClF_5O$ | 184.49 | 0.3 | | | | | | | | | 0.005 | | 0.008 | | | | | | | | 0.1 | | | |
| Isooctane / 2,2,4 Trimethylpentane | $C_8H_{18}$ | 114.23 | 0.009 | | | | | | | | 0.4 | 0.5 | | | | | | | | | | | | | |
| Isopentane / 2-Methylbutane | $C_5H_{12}$ | 72.15 | 0.006 | 0.4 | | | | | | | | | | | | | | | | | | | | | |
| Isopropyl acetate / 2-Propyl acetate | $C_5H_{10}O_2$ | 102.13 | m | | | | | | | | | s | | | s | | | | m | | | | | | |
| Isopropylbenzene / Cumene | $C_9H_{12}$ | 120.19 | m | | | | | | | | | | | m | | 0.7 | | | | | | | m | | |
| Limonene | $C_{10}H_{16}$ | 136.23 | 0.01 | | | | | | | | | | | | | | | | | 0.2 | 0.4 | | | | |
| Maleic anhydride | $C_4H_2O_3$ | 98.06 | | | | | | | | | m | | | | m | | | | | m | | | | | |
| Methane | $CH_4$ | 16.04 | 0.1 | | | | | | 0.2 | 0.4 | | | | | | | | | | | | | | | |
| Methanethiol / Methyl mercaptan | $CH_4S$ | 48.11 | 0.1 | | | | | | | | | | | 0.9 | | 1 | | | | | | | | | |
| Methanol | $CH_4O$ | 32.04 | 0.04 | | | | | | | | 0.5 | | | | 0.08 | | 0.2 | | | | | | | | |
| 2-Methoxyethanol | $C_3H_8O_2$ | 76.09 | m | 0.1 | | | | | | | | | 0.04 | 0.05 | | | | | | | | | | | |
| Methoxyflurane | $C_3H_4Cl_2F_2O$ | 164.97 | 0.05 | | | | | | | 0.04 | | | | 0.01 | | | | | | | | 0.03 | | | |
| 1-Methoxy-2-propanol | $C_4H_{10}O_2$ | 90.12 | s | | | | | | | | 0.06 | | 0.02 | 0.04 | | | | | | | | | | | |
| Methyl acetate | $C_3H_6O_2$ | 74.08 | 0.04 | | | | | | | 0.04 | | | | | 0.05 | | | | | | | | | | |
| Methyl acrylate | $C_4H_6O_2$ | 86.09 | 0.05 | | | | | | | | 0.02 | | | 0.1 | | | 0.2 | | | | | | | | |
| Methylamine | $CH_5N$ | 31.06 | 0.04 | 0.2 | | | | | | | | | | | | 0.6 | | | | | | | 0.2 | | |
| o-Methylanilin / o-Toluidine | $C_7H_9N$ | 107.15 | 0.05 | | | | | | | 0.1 | | | | | 0.4 | | | | | | | | | 0.1 | |
| Methylbiphenyl | $C_{13}H_{12}$ | 168.23 | s | | | | | | | | | m | | | | m | | | | | | | s | | |
| 2-Methylbutadien / Isoprene | $C_5H_8$ | 68.12 | 0.1 | | | | | | | | | | | | | | | | 0.4 | 0.3 | | | | | |
| 3-Methyl-1-butanol / Isoamyl alcohol | $C_5H_{12}O$ | 88.15 | s | s | | | | | | | | | | | m | | | | | | | | | | |
| 3-Methyl-2-butanone / Methyl isopropyl ketone | $C_5H_{10}O$ | 86.13 | 0.02 | | | | | | 0.2 | | | | | | | | | | 0.5 | | | | | | |
| 3-Methylbutyl acetate / Isoamyl acetate | $C_7H_{14}O_2$ | 130.19 | 0.02 | | | | | | | | 0.01 | | | | | 0.1 | | | | 0.9 | | | | | |
| Methyl tert-butyl ether | $C_5H_{12}O$ | 88.15 | 0.01 | | | | | | | | 0.04 | | | 0.05 | | | | | | | | | | | |
| Methyl chloroformate | $C_2H_3ClO_2$ | 92.50 | | | | | | | | | 0.04 | 0.01 | 0.02 | | | | | | | | | 0.2 | | | |
| Methylcyclohexane | $C_7H_{14}$ | 98.19 | 0.01 | | | | | | | 1 | | | | | | | | | | | | | | | |
| Methyl formate | $C_2H_4O_2$ | 60.05 | 0.03 | | | | | | | 0.03 | | 0.02 | | | | | | | | 0.3 | | | | | |
| 4-Methyl-3-heptanone | $C_8H_{16}O$ | 128.21 | s | | | | | | | | | | | m | | | m | | | | | | | | |
| Methylhydrazine | $CH_6N_2$ | 46.07 | 0.07 | 0.1 | | | | | | | | | | | | | | | | 0.2 | | | 0.3 | | |
| Methyl iodide | $CH_3I$ | 141.94 | 0.3 | | | | | | | 0.2 | | | | | | | | | | 1.3 | | | | | |
| Methyl isobutyl carbinol / 4-Methyl-2-pentanol | $C_6H_{14}O$ | 102.17 | s | | | | | | | | | | m | | m | | | | | m | | | | | |
| Methyl isobutyl ketone(MIBK)/4-Methyl-2-pentanone | $C_6H_{12}O$ | 100.16 | 0.02 | | | | | | | | | 0.08 | | | | | | | 0.1 | | | | | | |
| Methyl isopropyl ketone / 3-Methyl-2-butanone | $C_5H_{10}O$ | 86.13 | 0.02 | | | | | | 0.2 | | | | | | | | | | 0.5 | | | | | | |
| Methyl methacrylate | $C_5H_8O_2$ | 100.12 | 0.04 | | | | | | | | | 0.02 | | | | | | | 0.2 | | | | 0.6 | | |

| 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 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4-Methyl-2-pentanol / Methyl isobutyl carbinol | $C_6H_{14}O$ | 102.17 | s | | | | | | | | | | m | | m | | | | | m | | | | | |
| 2-Methylpropane / Isobutane | $C_4H_{10}$ | 58.12 | 0.01 | | | | | | | | | | 0.9 | | | | | | | | | | | | |
| 2-Methylpropene | $C_4H_8$ | 56.11 | 0.02 | | | | | | | | | | | | | | | | | 0.2 | 0.4 | | | | |
| 1-Methyl-2-pyrrolidone / N-Methylpyrrolidone | $C_5H_9NO$ | 99.13 | s | | | | | | 0.04 | | 0.2 | | | 0.3 | | | | | | | | | | | |
| Methylsalicylate | $C_8H_8O_3$ | 152.15 | 0.1 | | | | | | | | 0.02 | 0.03 | | | | | | | | | 0.7 | | | | |
| α-Methylstyrene | $C_9H_{10}$ | 118.18 | m | | | | | | | | | | | | | | | | | s | | | 0.5 | | s |
| 2-Methylstyrene | $C_9H_{10}$ | 118.18 | s | | | | | | | | | | | | | | s | | | m | | | s | | |
| Monomethylhydrazine | $CH_6N_2$ | 46.07 | s | | | | | | | | | | | | | s | | | s | | | | | m | |
| Morpholine | $C_4H_9NO$ | 87.12 | m | 0.04 | | | | | | | | | | | 0.2 | | | | | | | | 0.2 | | |
| Naphthalene | $C_{10}H_8$ | 128.17 | 0.07 | | | | | | | 0.5 | | | | | | | | | | | | | 0.06 | | |
| Nitrobenzene | $C_6H_5NO_2$ | 123.11 | | | | | | | | | | | | | 0.5 | | | | | | 0.3 | | | | |
| Nitroethane | $C_2H_5NO_2$ | 75.07 | m | | | | | | | | | | | | | | m | | | m | | | | | |
| Nitrogentrifluoride | $NF_3$ | 71.00 | | | | | | | | | | | | | 0.2 | | | 0.1 | | 0.2 | | | | | |
| Nitromethane | $CH_3NO_2$ | 61.04 | | | | | | | | | | | | 0.5 | | | | | | 0.7 | | | | | |
| 1-Nitropropane | $C_3H_7NO_2$ | 89.09 | m | | | | | | | | m | | | | | | | | | | | | m | | |
| 2-Nitropropane | $C_3H_7NO_2$ | 89.09 | 0.05 | | | | | | | | | | | 0.9 | | | | | | | 0.8 | | | | |
| Nitrosomorpholine | $C_4H_8N_2O_2$ | 116.12 | | 0.2 | | | | | | | | | | | 0.09 | | | | | | 0.9 | | | | |
| 3-Nitrotoluene / m-Nitrotoluene | $C_7H_7NO_2$ | 137.14 | w | | | | | | | | | | | 0.3 | | | | | | | | 0.3 | | | |
| Nitrous Oxide / Dinitrogen oxide | $N_2O$ | 44.01 | | | | | 0.03 | 0.5 | | | | | | | | | | | | | | | | | |
| Nonane | $C_9H_{20}$ | 128.26 | 0.007 | | | | | | 0.4 | | | | | | | | | | | | | | | | |
| Nonenal (Trans-2-nonenal) | $C_9H_{16}O$ | 140.22 | 0.03 | | | | | | | | | | 0.2 | | | | 0.5 | | | | | | | | |
| Novec 5110 | $C_5F_{10}O$ | 266.04 | | | | | | | | 0.003 | 0.004 | 0.007 | | | | | | | | | | | | | |
| Novec 7300 | $C_7H_3F_{13}O$ | 350 | | | | | | | | 0.002 | | 0.007 | | | | | 0.04 | | | | | | | | |
| Octane | $C_8H_{18}$ | 114.23 | 0.007 | 0.2 | | | | | | | | | | | | | | | | | | | | | |
| 1-Octanol | $C_8H_{18}O$ | 130.23 | 0.01 | | | | | | | | | | | 0.2 | | 0.2 | | | | | | | | | |
| 1-Octene | $C_8H_{16}$ | 112.21 | 0.01 | | | | | | 0.4 | | | | | | | | | | 0.2 | | | | | | |
| Pentanal | $C_5H_{10}O$ | 86.13 | 0.02 | | s | | | | 0.3 | | | | | | | | | | | | | | | | |
| Pentane | $C_5H_{12}$ | 72.15 | 0.01 | 0.3 | | | | | | | | | | | | | | | | | | | | | |
| 2-Pentanone | $C_5H_{10}O$ | 86.13 | 0.01 | | | | | | | | | 0.1 | 0.2 | | | | | | 0.8 | | | | | | |
| n-Pentyl acetate / Amyl acetate | $C_7H_{14}O_2$ | 130.19 | 0.02 | 0.7 | | | | | | 0.03 | | | | | 0.06 | | | | | | | | | | |
| Perfluoro-1,3-dimethylcyclohexane | $C_8F_{16}$ | 400.06 | | | | | | | | | s | | | | | | 0.06 | | | 0.07 | | | | | |
| Perfluoromethylcyclohexane | $C_7F_{14}$ | 350.05 | | | | | | | | | s | | | | | | 0.03 | | | 0.1 | | | | | |
| Phenol | $C_6H_6O$ | 94.11 | 0.6 | | | | | | | | | 0.008 | 0.1 | | 0.4 | | | | | | | | | | |
| Phenylhydrazine | $C_6H_8N_2$ | 108.14 | vw | | | | | | | m | | | | | | | | | | | | | | m | |
| 1-Phenylpropane | $C_9H_{12}$ | 120.19 | 0.02 | | | | | | 0.6 | | | | | | | | | | | | | | | | s |
| Phosgene / Carbonylchloride | $COCl_2$ | 98.92 | | | | | | | | | | | | | | | | | | | 0.02 | 0.02 | | | |
| Phosphine | $PH_3$ | 34.00 | | | | | | | | | | | | 0.3 | | 0.5 | | | | | | | | | |
| Phthalic anhydride | $C_8H_4O_3$ | 148.1 | | | | | | | | | | | | 0.2 | | | | | | 0.5 | | | | | 0.3 |
| α-Pinene | $C_{10}H_{16}$ | 136.23 | 0.009 | | | | | | | | | | | 0.4 | | | | | | | | | 0.6 | | |
| Propadiene | $C_3H_4$ | 40.06 | 0.8 | | | | | | | | | | | | | | | | | | 0.1 | | | | |
| Propane | $C_3H_8$ | 44.10 | 0.02 | 0.4 | | | | | | | | | | | | | | | | | | | | | |
| 1,2-Propanediol / Propylene glycol | $C_3H_8O_2$ | 76.09 | s | | | | | | | | | | | | 0.01 | | | | | | m | | | | |
| Propanoic acid | $C_3H_6O_2$ | 74.08 | 0.1 | | | | | | | | | | 0.03 | | | 0.3 | | | | | | | | | |
| Propanol | $C_3H_8O$ | 60.10 | s | 0.3 | | | | | | | | | | | 0.08 | | | | | | | | | | |
| 2-Propanol | $C_3H_8O$ | 60.10 | 0.02 | | | | | | | | | 0.09 | 0.07 | | | | | | 0.2 | | | | | | |
| Propene | $C_3H_6$ | 42.08 | 0.05 | | | | | | | | | | | | | | 0.4 | | | 0.3 | | | | | |
| n-Propyl acetate | $C_5H_{10}O_2$ | 102.13 | m | | | | | | | | s | | | | | m | | | | m | | | | w | |
| 2-Propyl acetate / Isopropyl acetate | $C_5H_{10}O_2$ | 102.13 | m | | | | | | | | | s | | | s | | | | m | | | | | | |
| Propylene glycol / 1,2-Propanediol | $C_3H_8O_2$ | 76.09 | s | | | | | | | | | | | | 0.01 | | | | | | m | | | | |
| Propylene glycol monomethyl ether acetate | $C_6H_{12}O_3$ | 132.16 | | | | | | | | | 0.01 | | 0.02 | 0.03 | | | | | | | | | | | |
| Propylene oxide | $C_3H_6O$ | 58.08 | s | | | | | | | | | | 0.7 | | | | | | | | | 0.2 | | | |
| Propyl nitrate | $C_3H_7NO_3$ | 105.09 | s | | | | | | | | | | | | | | s | | s | | | | | m | |

| Name | Brutto-formula | Molec.-weight | 987<br>3.4<br>2950 | 986<br>3.6<br>2800 | 989<br>3.7<br>2750 | 983<br>4.4<br>2270 | 985<br>4.5<br>2215 | 984<br>4.7<br>2150 | 968<br>7.7<br>1291 | 969<br>8.0<br>1254 | 970<br>8.2<br>1217 | 971<br>8.5<br>1179 | 972<br>8.8<br>1139 | 973<br>9.1<br>1101 | 974<br>9.4<br>1061 | 936<br>9.8<br>1020 | 975<br>10.2<br>981 | 988<br>10.6<br>946 | 976<br>10.6<br>941 | 977<br>11.1<br>900 | 978<br>11.6<br>861 | 979<br>12.2<br>822 | 980<br>12.8<br>783 | 981<br>13.4<br>746 | 982<br>14.1<br>710 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Propyne / Methylacetylene | $C_3H_4$ | 40.06 | 0.06 | | | | | | | 0.4 | | | | | | | | | | | | | | | |
| Pyridine | $C_5H_5N$ | 79.10 | 0.4 | | | | | | | | | | | | | 0.7 | | | | | | | | 0.3 | |
| Selenium hexafluoride | $SeF_6$ | 192.95 | | | | | | | | 0.4 | | | | | | | | | | | | | 0.01 | | 0.2 |
| Sevoflurane | $C_4H_3F_7O$ | 200.06 | 0.08 | | | | | | | | 0.006 | | 0.01 | | | | | | 0.2 | | | | | | 0.3 |
| Silane | $SiH_4$ | 32.12 | | | | | | | | | | | | | | | | s | | m | | | | | |
| Silicon tetrafluoride | $SiF_4$ | 104.08 | | | | | | | | | | | | | 0.03 | 0.02 | | | | | | | | | |
| Styrene | $C_8H_8$ | 104.15 | 0.1 | | | | | | | | | | | | | | | | 0.3 | | | | 0.2 | | |
| Sulfur dioxide | $SO_2$ | 64.06 | | | | | | | | | | 0.4 | 0.3 | | | | | | | | | | | | |
| Sulfur hexafluoride | $SF_6$ | 146.06 | | | | | | | | | | | | | | | 0.009 | 0.006 | 0.004 | | | | | | |
| 1,1,2,2-Tetrabromoethane | $C_2H_2Br_4$ | 345.65 | vw | | | | | | | | | m | | | | | | | | s | | | | m | |
| 1,1,2,2-Tetrachloroethane | $C_2H_2Cl_4$ | 167.85 | | | | | | | | | 0.2 | | | | | | | | | | | 0.1 | | 0.06 | |
| Tetrachloroethene | $C_2Cl_4$ | 165.83 | | | | | | | | | | | | | | | | | 0.04 | 0.07 | | | 0.2 | | |
| Tetrachloromethane | $CCl_4$ | 153.82 | | | | | | | | | | | | | | | | | | | | 0.03 | 0.02 | | |
| Tetraethylplumbane | $C_8H_{20}Pb$ | 323.44 | s | | | | | | | | | | 0.2 | | | | | | s | | | | | | |
| Tetrahydrofuran | $C_4H_8O$ | 72.11 | 0.01 | | | | | | | | | | | | 0.09 | | | 0.5 | | | | | | | |
| Tetrahydrothiophene | $C_4H_8S$ | 88.17 | 0.02 | | | | | | | | | m | | | | | | | | | 2 | | | | |
| Thionyl chloride | $Cl_2OS$ | 118.97 | | | | | | | | 0.02 | s | | | | | | | | | | | | | | |
| Thionyl fluoride | $F_2OS$ | 86.06 | | | | | | | | | | | | | | | | | | | | m | | 0.07 | s |
| Thiophene | $C_4H_4S$ | 84.14 | | | | | | | | s | | | | | | | | | | | m | | | | |
| Toluene | $C_7H_8$ | 92.14 | 0.05 | | | | | | | | | | | | 0.5 | | | | | | | | | 0.4 | 0.2 |
| 2,4-Toluenediamine | $C_7H_{10}N_2$ | 122.17 | w | | | | | | | | | m | | | | | | | | | | m | | | |
| 2,4-Toluene diisocyanate (TDI) | $C_9H_6N_2O_2$ | 174.16 | | | | | s | | | | | | | | m | | | | | | m | | | | |
| o-Toluidine / o-Methylanilin | $C_7H_9N$ | 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 | $C_6H_3Cl_3$ | 181.45 | | | | | | | | | | | | s | | 0.4 | | | | | | | s | | |
| 1,1,1-Trichloroethane | $C_2H_3Cl_3$ | 133.40 | 0.3 | | | | | | | | | | | 0.04 | | | | | | | | | | 0.08 | |
| 1,1,2-Trichloroethane | $C_2H_3Cl_3$ | 133.40 | 0.7 | | | | | | | | 0.4 | | | | | | | | 0.3 | | | | | 0.07 | |
| Trichloroethene | $C_2HCl_3$ | 131.39 | | 0.3 | | | | | | 0.4 | | | | | 4 | | | | 0.07 | | 0.08 | | | | |
| Trichloronitromethane / Chloropicrine | $CCl_3NO_2$ | 164.38 | w | | | | | | | 0.3 | | | | | | | | 0.4 | | 0.03 | | | | | |
| 1,2,3-Trichloropropane | $C_3H_5Cl_3$ | 147.43 | w | | | | | | | | m | | | | | | | | m | | | | | s | |
| Triethylamine (TEA) | $C_6H_{15}N$ | 101.19 | 0.02 | | | | | | | | 0.1 | | | | 0.1 | | | | | | | | | | |
| Trifluoromethyliodid | $CF_3I$ | 195.91 | | | | | | | | | s | | | 0.01 | | | | | | | | | | m | |
| Trimethylamine (TMA) | $C_3H_9N$ | 59.11 | 0.03 | 0.02 | | | | | | | | 0.2 | | | 0.1 | | | | | | | | | | |
| 1,2,4-Trimethylbenzene | $C_9H_{12}$ | 120.19 | 0.2 | | | | | | | | | | | | | 0.5 | | | | | | | 0.3 | | |
| 3,5,5-Trimethyl-2-cyclohexen-1-one / Isophorone | $C_9H_{14}O$ | 138.21 | 0.03 | 0.06 | | | | | | 0.1 | | | 0.5 | | | | | | | 0.5 | | | | | |
| 1,3,5-Trioxane | $C_3H_6O_3$ | 90.08 | w | 0.09 | | | | | | | | | | | 0.08 | | | | 0.09 | | | | | | |
| Undecane | $C_{11}H_{24}$ | 156.31 | 0.005 | 0.07 | | | | | | | | | | | | | | | | | | | | | |
| Vinyl acetate | $C_4H_6O_2$ | 86.09 | 0.4 | | | | | | | | 0.007 | | 0.03 | | | | | | | | 0.1 | | | | |
| Vinyl chloride | $C_2H_3Cl$ | 62.50 | | | | | | | | | | | | | | 0.4 | | | | 0.2 | | | | 0.4 | |
| m-Xylene | $C_8H_{10}$ | 106.17 | 0.03 | 0.7 | | | | | | | | | | | 0.9 | | | | | | | | 0.2 | 0.4 | |

Notification used in the chart:

= Measured detection limit – verified by Advanced Energy laboratory in Denmark

Normal = Calculated detection limit

Relative strenght of absorption band:

vw = very week
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/m³” by using equation (1) given in the box below.

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

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

**To Convert ppm to mg/m³ (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/m³:

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

**To convert measured gas concentrations from mg/m³ to ppm (at T °C and P atm.):**

Equation (1) can only be used to convert concentration units of a gas mea-sured 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 specifi ed 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 x $10^{-2}$ liter atm. $K^{-1}$ $mole^{-1}$
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:

*Detection limit = Detection limit in chart x DLF*

The factor DLF can be read in Table 1.

Example: Reading from the chart - the detection limit for Sulphur hexafluoride ($SF_6$) 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 SF6 (SIT of 0.5) = 0.006 ppm x 3.2 = 0.019 ppm
Detection limit SF6 (SIT of 50) = 0.006 ppm x 0.3 = 0.002 ppm

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