Quantitative Spectra Collection and Analysis for Spectral Library Formation Using a "Residual Gas Analyzer" compact Quadrupole Mass Spectrometer

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Abstract

Residual gas analyzers (RGAs) are compact quadrupole mass spectrometers used to identify gases remaining in a chamber at high vacuum. RGAs are often used qualitatively to identify gases based on observed mass-to-charge ratios (m/z). They can also be used to quantify gases and their partial pressures when properly calibrated. Accurate quantitative measurements require standard spectra of the compounds of interest and gas correction factors relating the total number of ions measured with the pressure of gas in the chamber. While spectra of pure compounds are relatively easy to obtain, gas correction factors are less easily measured due to the lack of direct pressure measurement methods at high vacuum. A method of obtaining standard RGA mass spectra and calculating gas correction factors using an Ideal Vacuum AnalyzaVac™ RGA high pressure kit is presented here. The RGA high pressure kit includes a manual variable leak valve which allows the RGA to safely sample a chamber at rough vacuum to atmospheric pressure. The higher pressure of the sample chamber is directly measured and the pressure inside the RGA is calculated using established mass transfer equations. The described method is applied to n-pentane as an example. This method was also applied to other common chemicals with results available through Ideal Vacuum's premium AutoZ⁺™ RGA software.

Introduction

Residual Gas Analyzers (RGAs) are compact mass spectrometers used in vacuum environments to identify the gases remaining in the chamber and measure their individual contributions to the chamber pressure. RGAs have a variety of applications and are used heavily in many industrial and scientific vacuum processes. They provide advanced leak detection and contaminant identification to troubleshoot chambers that are failing to achieve required vacuum levels. They are also used for outgassing analysis of plastics,[1] vacuum components, and cleaned surfaces that require a high degree of cleanliness and purity.[2] RGAs are often used in semiconductor fabrication[3,4] and high-performance coating applications for gas purity analysis and process monitoring during coating, deposition, and etching processes such as physical vapor deposition (PVD) and chemical vapor deposition (CVD).[5,6]

Leak detection and contamination analysis are usually qualitative techniques. The precise pressure of the leak or contaminant is less important than its identity and whether it is getting worse or better. For these applications, the RGA is actively monitored by a human who can visually identify and mentally gauge the quality of the mass spectrum. This has lead to RGAs being considered as mostly qualitative instruments by many professionals in the field. However, when properly calibrated, an RGA is capable of producing quantitative, reproducible measurements of gas partial pressures. This is especially useful for more precise, automated, and computationally demanding applications such as outgassing and purity analysis for mission critical components and processes.

In this paper, a method to calibrate an Ideal Vacuum AnalyzaVac high pressure RGA kit, collect spectra of a number of pure chemicals, calculate their ionization (gas correction) factors, and formulate a mass spectra reference library is described.

Theory

Most RGAs work according to the same principle of operation. Gas molecules at the RGA probe tip are ionized by electron impact ionization.[7] The electrons are typically generated thermionically by a hot, negatively biased tungsten or yttria-coated iridium filament similar to a Bayard-Alpert hot cathode gauge.[8] When the high energy electrons collide with gas molecules, energy is transferred to them resulting in ionization and fragmentation. While both positive ions (cations) and negative ions (anions) are created, positive ions are much more abundant in most situations and so most commercial RGAs only measure in positive ion mode.

The positively charged ions are accelerated through the RGA's quadrupole towards a detector. The quadrupole consists of four parallel metal rods that apply a mixture of constant direct current (DC) voltages and radio frequency alternating (AC) voltages. By choosing the correct voltages, ions of a single mass-to-charge ratio (m/z) are selected to pass through the quadrupole while all others are rejected.[9] Ions that successfully pass through the quadrupole filter are collected by the detector and converted into a current that is proportional to the ion's abundance or partial pressure. RGAs may be scanned across a range of m/z values to generate mass spectra of the gases inside the chamber.

The mass spectrum of a pure chemical compound generated by an RGA often contains many peaks, determined by the compound's isotope ratio, fragmentation pattern, ionization efficiency, and detection efficiency.

The isotope ratio of a chemical is substance dependent and will not change based on the instrument used. It is determined by the natural or synthetic abundances of multiple isotopes of the same element inside the chemical. For example, carbon occurs naturally in two isotopes: carbon-12, with a mass of 12 amu which has a 98.9% natural abundance, and carbon-13, with a mass of 13 amu and a natural abundance of 1.06%. Any ion that contains carbon from a natural source will have its peak split on a mass spectrum with a separation of 1 amu in a 98.9:1.06 ratio. Isotopic masses are not exactly amu integer values due to differences in nuclear binding energy. RGAs have a resolution of only 0.5 to 1 amu, therefore all isotopes are treated as having integer amu masses. The isotope ratio of a substance can be calculated using published isotopic abundance charts and forms the underlying pattern of its mass spectrum.[10–12]

The fragmentation pattern occurs when molecules are ionized by high energy electrons. Sometimes the molecules split, or fragment, into multiple smaller molecules and ions. Each molecule has a unique fragmentation pattern which is dependent on the electron energy. Higher energy electrons cause more fragmentation than lower energy electrons. The standard electron energy used for library RGA spectra is 70 eV.

The ionization efficiency is the ratio of ions formed due to electron impact ionization of a substance relative to nitrogen (N_2).[13] Nitrogen is the standard and is considered to have an ionization ratio of 1. Larger molecules and molecules with more atoms typically have ionization ratios greater than 1.

Detection efficiency is a measure of how well the RGA probe can transmit an ion through the quadrupole and detect it at its detector. Detection efficiency is heavily device dependent and is also a function of m/z.

The fragmentation pattern, ionization efficiency, and detection efficiency are all device dependent. Devices of the same manufacturer and model will only have small differences between devices. Similar RGAs made by different manufacturers will have larger discrepancies. However, these discrepancies can be minimized by choosing the same electron energy, properly calibrating the instrument to maintain constant and equal peak widths across the spectrum, and using full spectrum fitting techniques to average out differences in peak intensities. This allows use of library spectra across devices and manufacturers.

Procedure

Materials

The following chemicals were used to obtain standard RGA spectra: pentane (Sigma Aldrich, reagent grade, 98%), acetone (Sigma Aldrich, suitable for HPLC, ≥ 99.9%), diethyl ether (Sigma Aldrich, suitable for HPLC, 99.9%, inhibitor free), tetrahydrofuran (Sigma Aldrich, anhydrous, ≥ 99.9%), hexane (Sigma Aldrich, ReagentPlus®, ≥ 99%), cyclohexane (Sigma Aldrich, suitable for HPLC, ≥ 99.7%), benzene (Sigma Aldrich, suitable for HPLC, ≥ 99.9%), methanol (Sigma Aldrich, suitable for HPLC, ≥ 99.9%), acetonitrile (Sigma Aldrich, suitable for HPLC, gradient grade ≥ 99.9%), ethyl acetate (Sigma Aldrich, anhydrous, 99.8%), isopropanol (Sigma Aldrich, suitable for HPLC, 99.9%), ethanol (Sigma Aldrich, 200 proof, anhydrous, ≥ 99.5%), 1,4-dioxane (anhydrous, 99.8%, contains ≤ 25 ppm BHT as stabilizer), toluene (Sigma Aldrich, suitable for HPLC, 99.9%), n-propanol (suitable for HPLC, ≥ 99.9%), distilled water.

Setup

The RGA high vacuum chamber setup consisted of an Ideal Vacuum AnalyzaVac 100 amu RGA (**P1013456**) with its probe inserted into a stainless steel pumping manifold (**P1013473**) and connected via a CF 2.75” copper gasket (**P102278**) and bolt kit (**P104378**). The RGA was controlled, and pressure readings and spectra were obtained from the RGA using Ideal Vacuum’s AutoZ⁺™ software. The pumping manifold was connected to an Agilent TPS-Mini TwisTorr 74FS turbomolecular pumping station with built-in diaphragm pump (**P103100**) via a CF 4.5” copper gasket (**P102280**) and bolt kit (**P104377**). The pumping manifold was extended with a CF 2.75” tee (**P102193**) via a CF 2.75” copper gasket and bolt kit. The tee was connected to an Agilent manual

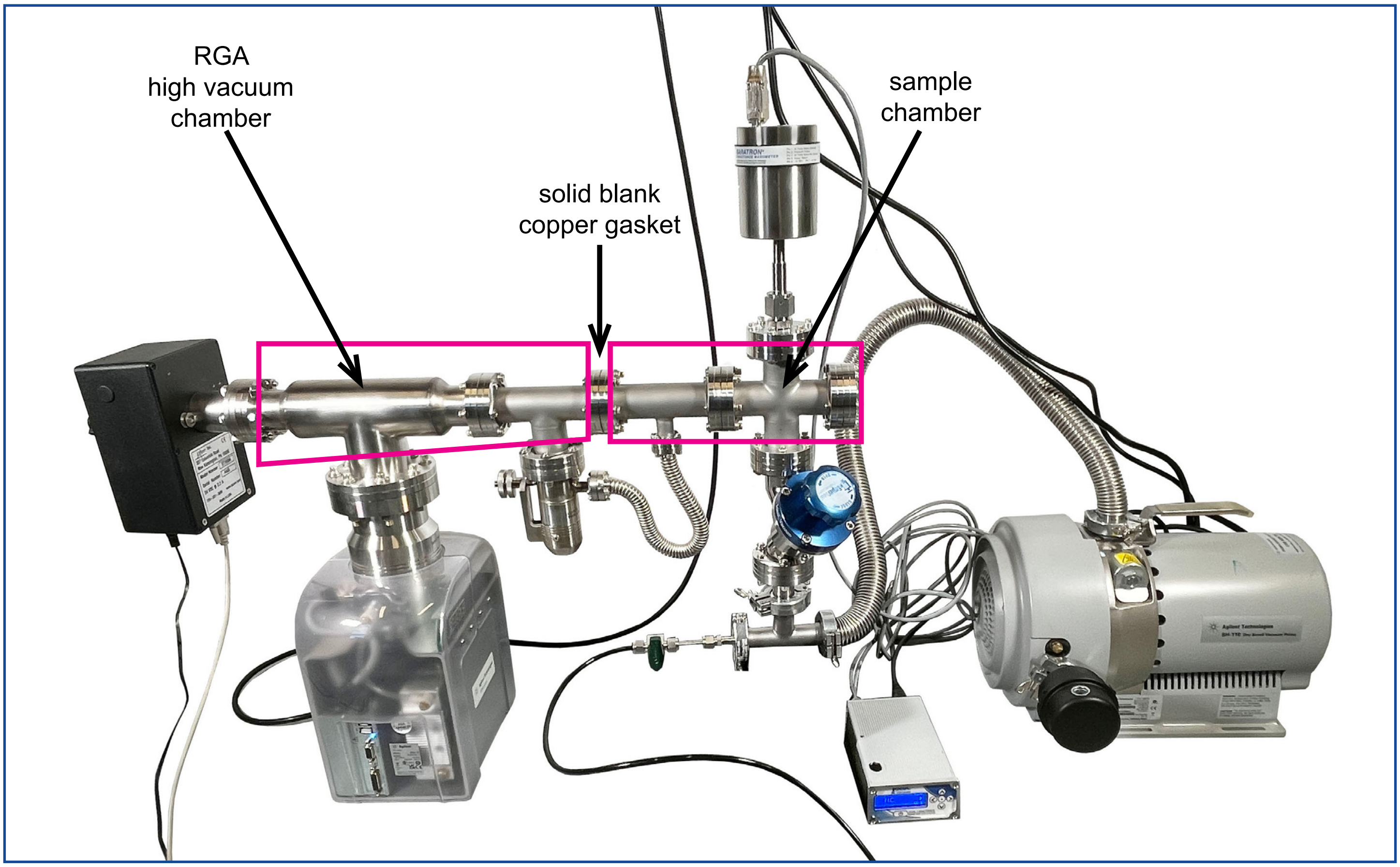

__Figure 1:__ Photograph of RGA library collection setup with background removed.

variable leak valve (**P105211**) via a CF 2.75” copper gasket and bolt kit. This constituted a prototype of the AnalyzaVac 100 amu manual high pressure kit (**P1013472**). This RGA high vacuum chamber setup was used for all compounds with molecular ions of mass less than 100 amu.

For compounds with molecular ions of mass greater than 100 amu, an AnalyzaVac 300 amu RGA (**P1013459**) was substituted into the same setup.

The sample chamber consisted of a CF 2.75” cross (**P102185**) connected to a CF 2.75” to CF 1.33” reducing tee (**P104850**). The reducing tee was attached to the RGA high pressure kit structurally via its remaining CF 2.75” flange with a leak-tight solid blank copper gasket (**P104350**) and bolt kit. It was connected to the manual leak valve inlet via a 12” CF 1.33 flexible bellows (**P102226**) with CF 1.33” copper gaskets (**P102277**) and bolt kits (**P104397**).

One of two MKS Baratron® capacitance manometer gauges were connected to the sample chamber via a CF 2.75” to VCR 8 male adapter (**P102266**) with a 316L VCR 8 retained gasket (**P1013249**). For chemicals with vapor pressures greater than 2 Torr, a model 627H 1000 Torr Baratron capacitance manometer (**P1012585**) was used. For pressures below 2 Torr, a model 628B 2 Torr Baratron was used. Pressures were displayed using an Ideal Vacuum dual capacitance manometer gauge controller (**P1010127**). Samples were injected into the chamber through a custom rubber septum port on the CF 2.75” cross. The chamber was connected to an Ideal Vacuum Super-Seal™ CF 2.75” inline manual bellows valve (**P1011847**), then adapted to a KF-25 tee. An Agilent SH-110 dry scroll rough vacuum pump and a nitrogen gas manifold were connected to the tee.

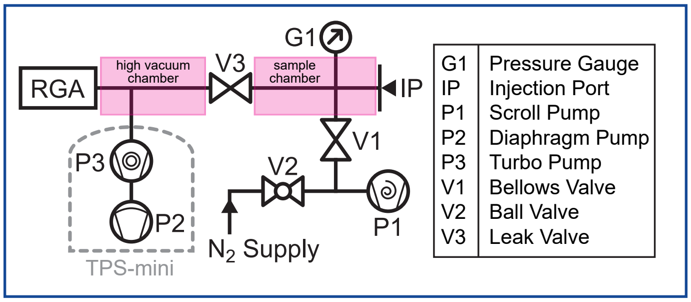

Figure 2: *System diagram of RGA library collection setup.*

Calibration

To obtain a pressure below the minimum pressure of the gauge, after the capacitance manometer gauge controller read 0 pressure, the sample chamber was evacuated for an additional 15 minutes and the controller was zeroed. Then, the chamber was vented to atmospheric pressure and the controller full scale multiplier was adjusted to 0.99 to match the correct pressure. The capacitance manometer and pressure controller were now properly calibrated.

The RGA was calibrated according to the full calibration procedure described in the AutoZ$^+$ RGA software user manual. In summary, the electron energy was set to 70 eV, the standard for RGA spectra. The high and low calibration offsets and resolutions were adjusted to obtain peaks centered ±0.07 amu from integer values with 1 amu full peak width at 10% peak height across 2-100 amu for the 100 amu RGA unit and 2-300 amu for the 300 amu unit. Several compounds of known spectra were injected to verify that the peaks were of correct intensity across the m/z measurement range without systematic error based on m/z value. This was found to be true without adjusting the ion energy, which was set at 5 eV across the full spectrum range, as expected of new and lightly used RGA units.

The RGA was then flooded with pure nitrogen gas and the partial sensitivity was calibrated so that the sum of the partial pressures (the “corrected” pressure in AutoZ$^+$) matched the total pressure measured by the RGA’s built-in hot cathode ion gauge (the “gauge pressure in AutoZ$^+$). The hot cathode ion gauge was factory calibrated to nitrogen and assumed to be correct. It is possible that even better results could be achieved by calibrating to a NIST certified hot cathode gauge.

To determine the relationship between sample chamber pressure and the RGA chamber pressure, the sample chamber was brought to 400 Torr of nitrogen gas, a pressure similar to the vapor pressure of the most volatile samples measured.

The RGA was actively pumped by the attached TPS-mini turbo package and brought below 1 × 10^{-8} Torr. The variable leak valve between the RGA and sample chamber was slowly opened while monitoring the RGA pressure to achieve an RGA pressure of 2.5 × 10^{-7} Torr, close to the RGA's optimal operating pressure. The variable leak valve was then set.

The sample chamber was then evacuated and the pressure raised in steps from 0 to 600 Torr. Using the AnalyzaVac's built-in hot cathode ion gauge, the pressure of the RGA was measured at each step. This procedure was repeated later to obtain new pressure calibration curves for less volatile molecules. Depending on the vapor pressure of the molecules to be tested, the initial sample chamber pressure was set to be 175, 100, and 50 Torr when the leak valve was set to obtain an RGA pressure of 2.5 × 10^{-7} Torr

Spectra Collection

Before each sample spectra collection the sample chamber was pumped out for at least 15 minutes to achieve baseline pressure according to the capacitance manometer gauge. The RGA pressure and spectra were also monitored. An RGA pressure less than 1 × 10^{-8} Torr and a static spectrum was required before advancing to the next step.

The bellows valve to the nitrogen and vacuum manifold was closed and baseline RGA spectra were averaged over ten minutes. If there was a detectable rate of rise in the pressure of the sample chamber, the rubber septum would be replaced and sample collection would be restarted.

A volume of up to 1 ml of a test compound was injected into the sample chamber using a 1 ml syringe. This volume was chosen to be sufficiently large that an equilibrium could be achieved between the gas and liquid phase of the sample and so that complete evaporation would not occur. After the injection, the needle was removed from the septum and the pressures of the RGA and sample chamber were allowed to reach steady state. The RGA then collected and averaged spectra of the sample over a period of at least 10 minutes.

Results and Discussion

A library RGA spectrum for quantitative analysis requires two things. The first is a spectrum of the compound. This is not difficult to obtain as it only requires some amount of sample to be measured by the RGA. The second requirement is a gas correction factor, or ionization factor, that correlates the total number of ions generated and a measurement of the compound's pressure at the RGA probe tip. This is not easily obtained because RGAs only work under high vacuum and there are few direct pressure measurement methods that are effective at high vacuum. Both hot cathode and cold cathode gauges, commonly used to measure pressure at high vacuum, require a gas correction factor to produce accurate results for any gas that is not primarily composed of nitrogen or oxygen. To overcome this, the pressure of the samples at high vacuum based on a nitrogen calibration and differences in diffusion speeds was calculated.

The RGA was separated from the sample chamber by a variable leak valve.[14] This allowed the RGA to operate at its optimal pressure, around 2 × 10^{-7} Torr, while the sample pressure in the sample chamber could be in the atmospheric to rough vacuum range. The sample pressure was measured by a capacitance manometer which directly measures pressure independent of sample identity. Capacitance manometers also have the advantage of providing highly linear, highly accurate, pressure readings with NIST traceable calibration. In this case, the capacitance manometer reading was only 1% different from the calibration value. This could be due to factors as small as electronic resistance in the signal carrying wire.

The leak rate, or rate of effusion, through the variable leak valve is a function of the difference in pressure between the RGA chamber and the sample chamber, and the average speed of the gas molecules. The pressure inside the RGA chamber was so small relative to the sample chamber pressure that its contribution is negligible. The sample chamber pressure remained effectively constant because the leak was very small relative to the total quantity of gas in the sample chamber. Also, enough sample was injected to allow some sample to remain in a liquid state, resulting in an equilibrium vapor pressure in the sample chamber. Even if a significant amount of sample vapor were removed, liquid sample would evaporate to maintain a constant pressure inside the sample chamber.

The ratio of effusion rates of two gases through the leak valve at the same pressure and temperature is well approximated by Graham's law for effusion shown in equation 1.

$$\frac{rate\ of\ effusion\ of\ A}{rate\ of\ effusion\ of\ B} = \sqrt{\frac{M_B}{M_A}}$$

Equation 1: Graham's law for effusion

Where M_B is the molar mass of compound B (g mol^{-1}) and M_A is the molar mass of compound B (g mol^{-1}).

The RGA chamber is constantly pumped by an Agilent TPS-mini turbomolecular pumping station. The pumping speed, S_{eff} (l s^{-1}), of a turbomolecular pump for heavy gases (molecular weight > 20) can be approximated by equation 2.

$$S_{eff} = \frac{Av}{4\left(\frac{v}{\bar{c}} + 1\right)}$$

Equation 2: Turbomolecular pump effective pumping speed

Where A is the area of the pump inlet, *v* is the turbo pump blade radial velocity (m s^{-1}), and c is the average molecular velocity (m s^{-1}) given by equation 3.[15]

$$\bar{c} = \sqrt{\frac{8RT}{\pi M}}$$

Equation 3: Average speed of gas molecules

Where R is the ideal gas constant, 8.31447 J mol^{-1} K^{-1}, T is the temperature (K), and M is the molecular weight of the gas (kg mol^{-1}).

When a leak is introduced into the RGA chamber through the variable leak valve, the pressure inside the RGA chamber rises until the leak rate into it equals the clearance rate through the turbomolecular pump. This produces a steady state pressure inside the RGA chamber (P_{RGA}) that obeys equation 4.

$$P_{RGA} * S_{eff} = rate\ of\ effusion$$

Equation 4: Steady state RGA pressure rate equation

Taking the ratio of the steady state RGA pressure of a substance of unknown pressure, $P_{RGA,Sub}$, with the steady state RGA pressure of nitrogen, $P_{RGA,N2}$ grants equation 5.

$$\frac{P_{RGA,Sub} * S_{eff,Sub}}{P_{RGA,N_2} * S_{eff,N_2}} = \frac{Rate\ of\ effusion\ of\ substance}{Rate\ of\ effusion\ of\ N_2} = \sqrt{\frac{M_{N_2}}{M_{Sub}}}$$

Equation 5: Ratio of substance pressure to nitrogen pressure inside RGA chamber

Solving for $P_{RGA,Sub}$ grants equation 6.

$$P_{RGA,Sub} = P_{RGA,N_2} * \sqrt{\frac{M_{N_2}}{M_{Sub}}} * \left(\frac{v * \sqrt{\frac{\pi M_{sub}}{8RT}} + 1}{v * \sqrt{\frac{\pi M_{N_2}}{8RT}} + 1}\right)$$

Equation 6: RGA chamber pressure of a substance

The velocity of the turbo blade, *v*, differs from its center to its edge, so a mean blade velocity is used as shown in equation 7.

$$v = \pi f(r_i + r_o)$$

Equation 7: Mean turbo blade velocity

Where f is the frequency of the turbo blade spinning (Hz), r_i is the inner radius of the turbo blade (m), and r_o is the outer radius of the turbo blade (m). For an Agilent 74 FS, the turbo blade frequency is 81000 RPM (1350 Hz), the blade inner radius is 20.0 mm (0.0200 m), its outer radius is 32.5 mm (0.0325 m), and the blade velocity is 223 m s^{-1}.

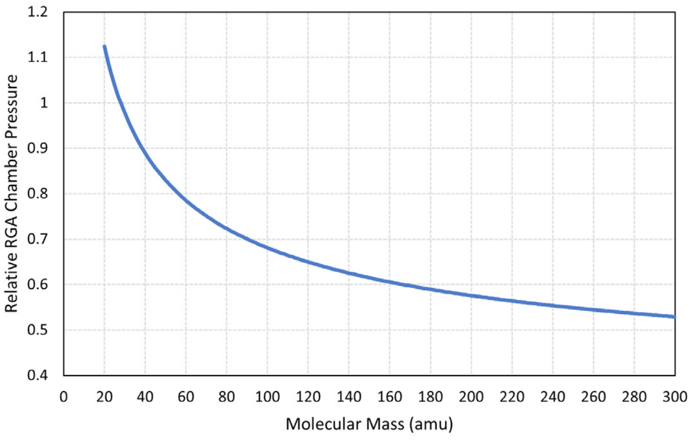

Figure 1: RGA chamber pressure relative to nitrogen gas (N_2) as a function of gas molecular mass assuming equal sample chamber pressure, T = 290.65 K, and an Agilent 74 FS turbo pump.

Armed with this information, the relative RGA chamber pressure of a substance compared to nitrogen can be calculated as long as both the substance and the nitrogen have the same pressure and temperature and the substance's molecular mass is known. A graph of the relationship between molecular mass and RGA chamber pressure relative to nitrogen gas is shown in Figure 1. Substances of molecular mass less than nitrogen have higher pressures than nitrogen inside the RGA chamber and substances of molecular mass greater than nitrogen have lower pressures for the same sample chamber pressure.

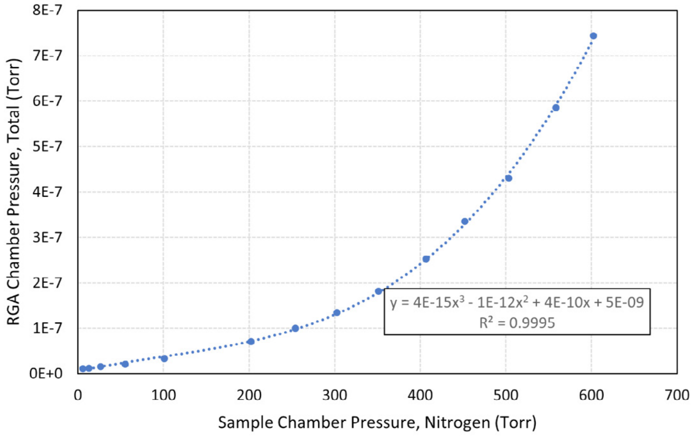

Figure 2: Total RGA chamber pressure as a function of sample chamber nitrogen gas pressure (blue dots) and third order polynomial fit (blue dashed line). The leak valve was originally set to yield an RGA pressure of 2.53×10^{-7} Torr with a sample chamber pressure of 406 Torr.

It is difficult to exactly match sample pressure to nitrogen pressure in the sample chamber. However, the relationship between sample chamber nitrogen pressure was measured at several different leak valve crack points. A simple polynomial fits the data well. An example is shown in Figure 2.

For example, pentane has molecular formula C_5H_{12} and an average molecular weight of 72.15 amu. By applying equation 6 for the test conditions shown in Figure 1, the pressure of pentane inside the RGA chamber should be 74% of the pressure of nitrogen given the same sample chamber pressure of nitrogen. The pressure of pentane in the sample chamber was 376 Torr, close to the expected value of 388 Torr.[16] Using the fit shown in Figure 2, the expected contribution of nitrogen to the RGA chamber due to an external pressure of 376 Torr would be 2.03×10^{-7} Torr, yielding a calculated pentane pressure inside the RGA of 1.51×10^{-7} Torr.

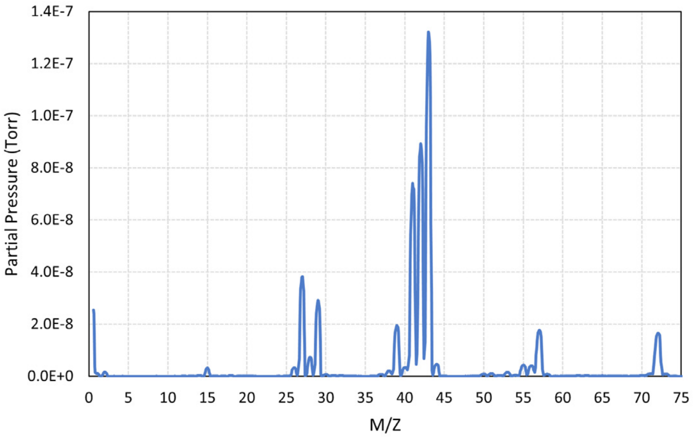

Figure 3: Analog RGA spectrum of 1.51×10^{-7} Torr of pentane

Figure 3 shows an analog mass spectrum of pentane obtained at the pressure calculated above. The RGA high vacuum chamber always has some amount of residual gas in it, even when closed off to the sample chamber. This is due to imperfect pumping, lack of bakeout, oxidation of the carbon in steel, and migration of hydrogen through the steel chamber walls.

When the RGA has been pumped for a significant amount of time, the residual gas is primarily composed of water, hydrogen, and carbon dioxide. A mass spectrum of the residual gases in the RGA when well pumped out is shown in Figure 4.

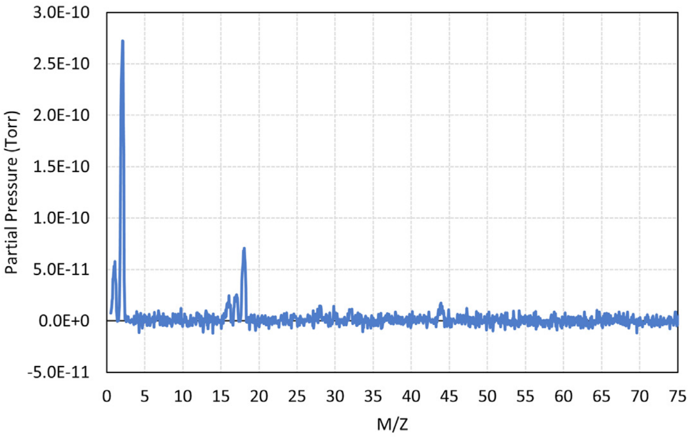

Figure 4: Analog RGA spectrum of a closed, well pumped out RGA chamber. The peaks at 1 and 2 amu are from hydrogen, the peaks at 16, 17, and 18 amu are from water, and the peak at 44 amu is from carbon dioxide. No other peaks or gases are distinguishable above the noise floor of approximately 1×10^{-11} Torr.

The pressure of these residual gases is small, on the order of 10^{-10} Torr, relative to the pressure of the sample. However, we removed their contribution to the spectrum by collecting and subtracting a spectrum of the residual gases immediately before introducing the sample into the RGA chamber. This produced spectra of the pure sample gas without contributions from other gases.

The peak locations and relative intensities of pentane were tabulated to make a standard spectrum. A standard spectrum defines the positions and relative intensities of all significant spectrum peaks of a pure compound obtained under standard conditions. Peaks were assigned to integer amu values because the resolution of the RGA and the possibility of thermal drift make more precise measurement non-useful. Pentane consists of only carbon and hydrogen atoms, so the chemical formula of the ion fragments producing each peak were easily deduced.

Mass	Formula	Relative Intensity (%)
1	H^+	1.14
2	H_2^+	1.22
15	CH_3^+	2.37
27	$C_2H_3^+$	28.88
28	$C_2H_4^+$	5.48
29	$C_2H_5^+$	22.00
30	$C_2H_6^+$, $^{13}CCH_5^+$	0.51
37	C_3H^+	0.58
38	$C_3H_2^+$	1.51
39	$C_3H_3^+$	14.77
40	$C_3H_4^+$	3.04
41	$C_3H_5^+$	56.01
42	$C_3H_6^+$	67.50
43	$C_3H_7^+$	100.00
44	$C_3H_8^+$, $^{13}CC_2H_8^+$	3.46
50	$C_4H_2^+$	0.63
51	$C_4H_3^+$	0.80
53	$C_4H_5^+$	1.16
54	$C_4H_6^+$	0.27
55	$C_4H_7^+$	3.21
56	$C_4H_8^+$	3.02
57	$C_4H_9^+$	13.39
58	$C_4H_{10}^+$, $^{13}CC_3H_9^+$	0.60
71	$C_5H_{11}^+$	0.74
72	$C_5H_{12}^+$ (pentane)	12.50
73	$^{13}CC_4H_{12}^+$	0.69

Table 1: Tabulated standard mass spectrum of pentane generated by an AnalyzaVac RGA using standard calibration values.

The spectrum shows a molecular ion peak with moderate intensity at 72 amu. However, the most intense peak arises from a $C_3H_7^+$ fragment. Interestingly, the peaks arriving from non-radical cations, such as the propyl cation, $C_2H_3^+$, at 27 amu, and ethyl cation, $C_2H_5^+$, at 29 amu, are typically more intense than peaks arising from radical cations such as $C_2H_4^+$ at 28 amu. While these general trends may be predictable by a trained spectroscopist, the full spectrum with many fragments is not accurately predictable using current technology. However, the spectrum is repeatable, and once experimentally obtained, may be used as a library reference.

Ionization (Gas Correction) Factor

The pressure readings of the RGA spectrum are calibrated to nitrogen gas such that the sum of the pressures of the peaks created by nitrogen at 14 and 28 amu is equal to the total pressure of nitrogen in the RGA chamber.

This is not necessarily true for other compounds. In order to accurately measure the total pressure of a compound other than nitrogen, an ionization factor, or gas correction factor, is required to correlate the total measured pressure of all ions produced by a substance to the RGA chamber pressure of the substance as descibed in equation 8.

$$GCF_A = \frac{\sum p_A}{\sum p_{N_2}}$$

Equation 8: Calculation of ionization (gas correction) factor

Where GCF_A is the gas correction factor of substance A, P_A are a collection of all measured partial pressure values of A at different m/z values at a given total pressure of A, and P_{N_2} are a collection of all measured partial pressure values of N_2 at different m/z values at the same total N_2 pressure as A. For an instrument calibrated for nitrogen, the sum of P_{N_2} is equal to the total pressure of A.

For pentane, the RGA chamber pressure was 1.51×10^{-7} Torr, but the total measured pressure of all ions was 4.57×10^{-7} Torr. This yields an ionization factor of 3.02 for pentane.

Conclusion

A standard RGA mass spectrum of n-pentane was obtained using an Ideal Vacuum AnalyzaVac RGA with default acquisition parameters. A total of 26 peaks were observed with m/z values ranging from 1 to 73 amu. The two most notable peaks were the largest peak at 43 amu, corresponding to the propyl cation, and the molecular ion at 72 amu. A gas correction factor, or ionization factor, of 3.02 was measured for pentane, meaning that pentane produces 3.02 times more positive ions than an equivalent pressure of nitrogen under the same conditions. This makes intuitive sense because n-pentane has a much larger ionization cross section than nitrogen.

Measurement of the gas correction factor for n-pentane required a two-chamber system. Pentane was injected into a sample chamber at rough vacuum. A small amount of the sample gas was allowed to travel through the leak valve into the high vacuum chamber (the AnalyzaVac RGA high pressure kit).

The pressure of pentane in the sample chamber was directly measured using a capacitance manometer. The rate of effusion through the variable leak valve connecting the chambers and the resulting RGA chamber pressure were calculated using a nitrogen calibration curve, Graham's law of effusion, and the mass-dependent turbomolecular pumping speed.

The process was repeated for 15 other commonly used chemicals. Those results are included as part of the substance library included with the premium version of Ideal Vacuum's AutoZ+ RGA software. AutoZ+ uses full-spectrum least squares analysis to provide quantitative measurement of partial pressures of gases included in its substance library.

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