

TECHNICAL NOTE

How to Use the NIST Spectra Library

Residual Gas Analyzers (RGAs) have been used in vacuum research applications for 25 years. Their role has changed in the last 10 years, as they have evolved from purely a research instrument to a production tool. As a production tool, the RGA can increase productivity, improve product yield, increase throughput and reduce costs, all of which ultimately increase profits.

An RGA is a commonly used tool for identifying the residual gases in a vacuum chamber. In the RGA, residual gases are ionized, separated by mass-to-charge, and plotted based on their ion intensities as a mass spectrum. The mass-to-charge values are unique for each gas species, and therefore, each chemical substance has a characteristic mass spectrum. When gas mixtures are analyzed, it is sometimes difficult to identify which gas species are within the process. For example, the peak at mass 28 could be either nitrogen or carbon monoxide. With the help of a mass spectra library, the RGA can determine which gases might be contributing to specific mass peaks.

FRAGMENTATION PATTERN

The mass spectrum obtained when the parent molecule breaks apart under electron impact is commonly referred to as the fragmentation pattern (or cracking pattern). This fragmentation pattern forms a fingerprint that may be used for identification of a gas or vapor molecule. The more complex the molecule, the more complex the fragmentation pattern. There are two other characteristics which contribute to the various peaks: isotope ratios and multiple ionization.

ISOTOPE RATIOS

The Atomic Mass Unit (AMU) of an element is the number of naturally occurring protons and neutrons. An isotope of an element occurs with the addition or subtraction of one or more neutrons from its natural element. These isotope ratios are a very useful aid in recognizing specific materials. Under normal ionization conditions, the peak height ratios for the various isotopes of an element will be the same as the ratios of their

natural abundance. Using Argon as an example, the main or parent peak for Argon is seen at AMU 40 (22 neutrons and 18 protons), while there are isotopes of Ar at AMU 36 (18 neutrons and 18 protons) and AMU 38 (20 neutrons and 18 protons).

MULTIPLE IONIZATION

When an electron with sufficient energy strikes a gas molecule, many processes can occur. Sometimes more than one electron is stripped off the molecule. This newly created ion passes through the mass filter and will have a charge of ++ rather than just +. If the gas is Ar for example, the major signal reaching the collector will be Ar^+ , but there will be some Ar^{++} as well. The presence of both Ar^+ and Ar^{++} is called the fragmentation pattern of Argon. An RGA displays mass-to-charge ratios on its X-axis. A single ionized parent Ar molecule, Ar^+ , will be displayed at a mass-to-charge ratio of $40 / + 1 = 40$. A double charged Ar molecule, Ar^{++} , will be displayed at a mass-to-charge ratio of $40 / + 2 = 20$.

While mass-to-charge values are unique for each gas species, the peak amplitudes are dependent on the gas and instrumental conditions. The height of a peak in a mass spectrum is proportional to the partial pressure of ions giving rise to that peak. Partial pressure is defined as the pressure of a designated component in a gas mixture. The relative amplitudes of the gas (molecule) are determined by the gas source and the instrument. Therefore, different instruments will give slightly different spectra for the same substance. Also, the ion energy and electron energies affect the probability of dissociation and the formation of higher ionization states.

USING THE NIST SPECTRAL LIBRARY

The NIST Mass Spectral Library contains mass spectra and associated information for compounds. The main collection contains a single spectrum for each compound and is developed to provide reliable mass spectral "fingerprints" to assist in the identification of compounds. The fragmentation pattern and other information can be obtained through the

NIST website, <http://webbook.nist.gov/chemistry/>. The NIST Chemistry WebBook provides users with easy internet access to chemical and physical property data for chemical species. The data provided in the site are from collections maintained by the NIST Standard Reference Data Program and outside contributors. Data in the WebBook system are organized by chemical species. For all species, a set of general information is displayed at the top of the page. This information includes: species name, molecular weight, CAS (Chemical Abstract Service) registry number (if available), structure image (if available), mass spectrum, links to other data, option for changing the system of units.

SEARCHING FOR CHEMICAL SPECIES

The NIST Chemistry WebBook supports several types of direct searches for chemical species. The available search types are formula, chemical name, ionization energy, electronic energy level, molecular weight, proton or electron affinity, etc. For example, if the chemical formula search is used (the results of which are seen in figs. 1 and 2), you are prompted to enter the desired chemical formula.

Rules for Using Chemical Formulas:

- Elements may be in any order, but correct case for element symbols must be used. Otherwise, the formula may be ambiguous, and the interpretation chosen may not be the desired one.
- To specify any letter of a given element, use a question mark (?) after the element symbol.
- To specify any number of a given element, use an asterisk (*) after the element symbol. To explicitly specify an ion, place the charge at the end of the formula (e.g., C60⁻²).
- Each search option has its own rules, which are explained under search help in the selected search page.

Each of the direct search types allow the user to select the units to be applied when displaying the data (fig. 2). The user may choose between SI units and calorie-based units. Choosing the latter will result in energy and pressure values displayed in calories and atmospheres rather than Joules and bars. If a search finds more than one chemical species that match the search criteria, the matching species will be displayed on a selection page.

Most of the search types discussed above share several common features, including: the ability to select the units to be used, the ability to select the types of data to be displayed, and a common format for displaying the results of a search where more than one species match the search criterion.

Using the NIST Website is an easy method for identifying unknown compounds that may be relevant to your analysis.

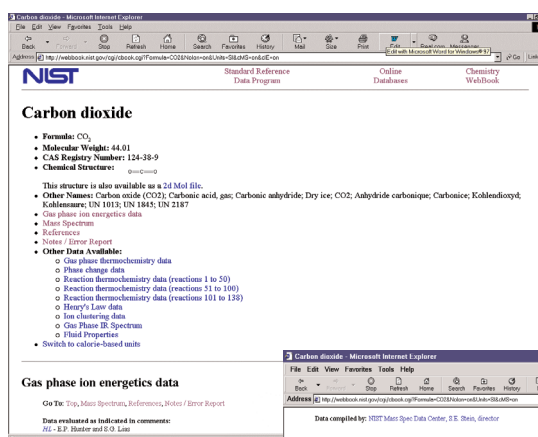


Figure 1 - CO₂ output using formula search.

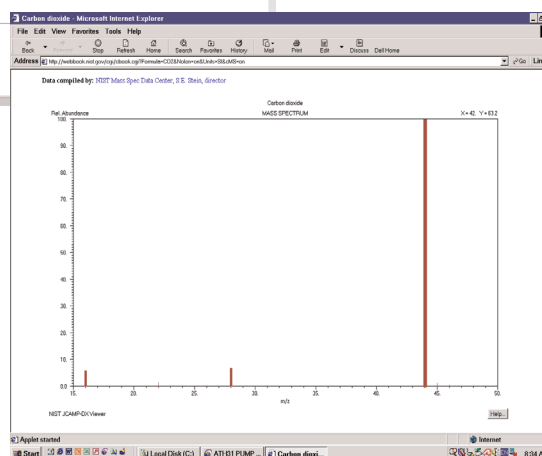


Figure 2 - Fragmentation pattern of CO₂.



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