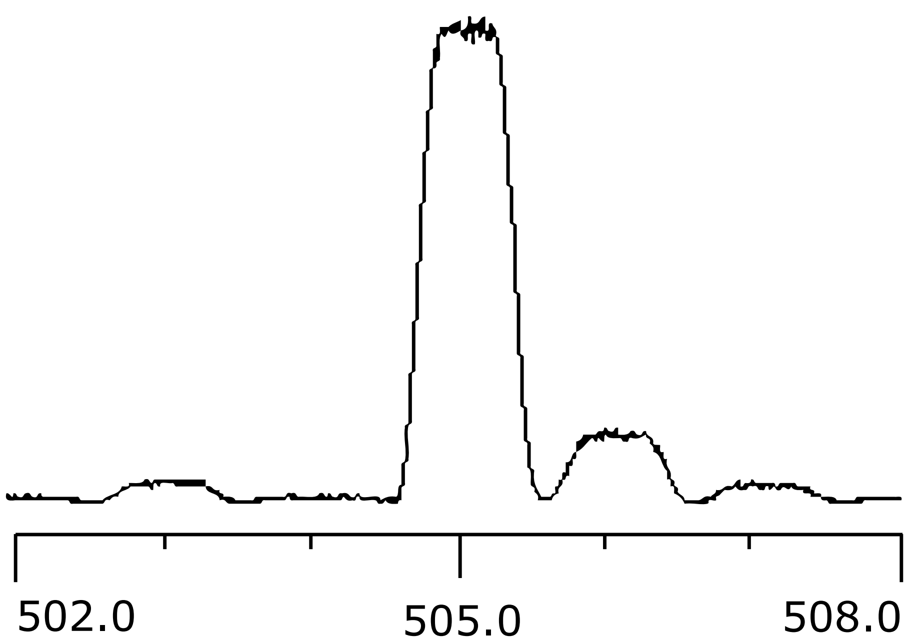
Mass Spectrometers

How Resolution is Defined

Several different definitions of resolution are used in mass spectrometry. It is useful to understand the distinctions between the different definitions to understand the characteristics of different mass spectrometers.

Unit resolution means that you can separate each mass from the next integer mass. That is, you can distinguish mass 50 from mass 51, and you can distinguish mass 1000 from mass 1001. This definition is commonly used when discussing resolution on quadrupole and ion trap mass spectrometers. Peak shapes in quadrupole mass spectrometers are usually "flat-topped".

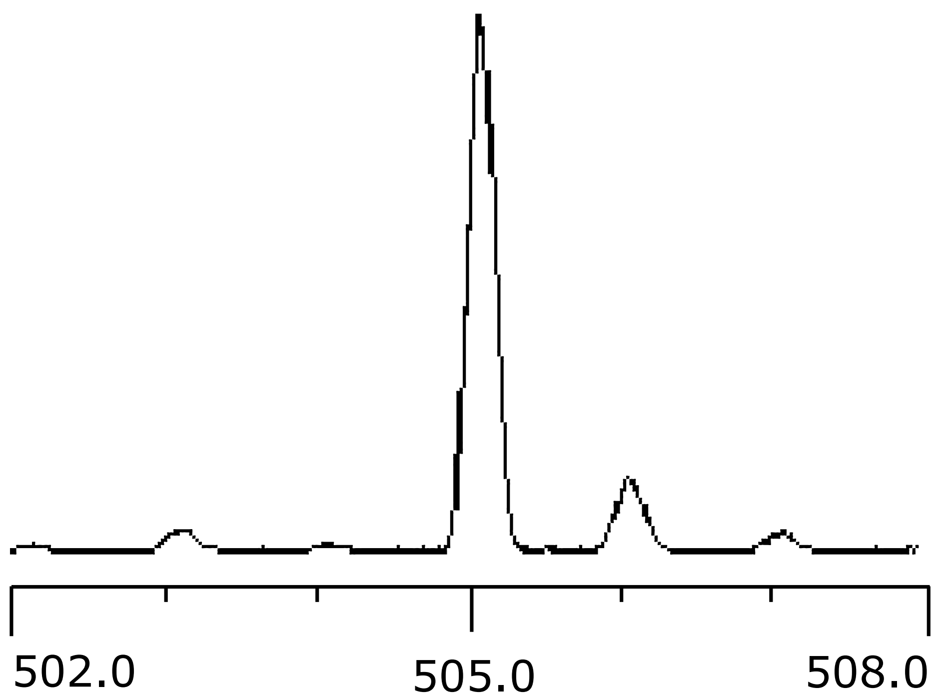


Flat-topped peaks, roughly unit resolution at m/z *500*

Magnetic sector mass spectrometers define **resolving power** as:

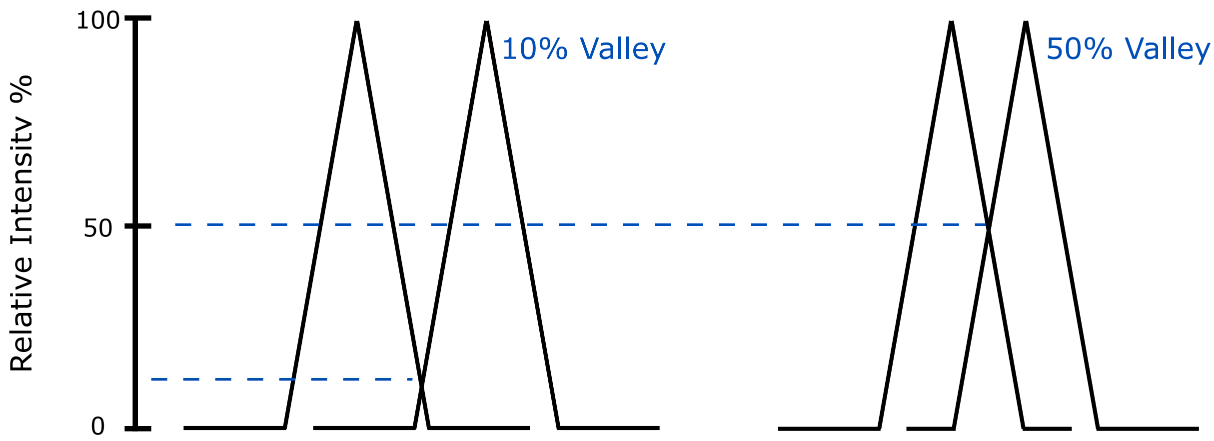
$$R = \frac{m}{\Delta m}$$

that is, the the mass number of the observed mass divided by the difference between two masses that can be separated. Magnetic sector mass spectrometers have peak shapes that are triangular or Gaussian.



Peak shapes from a magnetic sector MS (resolving power ~ 1,000)

In magnetic sector mass spectrometers, peaks are usually defined to be separated down to a *10% valley*, that is, a point that is 1/10 of the height of the higher of the two peaks. If you only have one peak, then you can estimate the resolving power by using the peak width at the 5% level divided by the mass of the observed peak. The resolving power value as defined above is



Two peaks resolved to 10% valley (left) and 50% valley (right)

constant across the mass range. The 10% valley definition is usually considered adequate for resolving small isotope peaks.

Fourier transform ion cyclotron resonance (FTICR) mass spectrometers use the same resolving power definition as magnetic sector mass spectrometers. However, it is common to use a 50% valley definition for the resolution because of the broadening near the baseline of the unapodized magnitude-Lorentzian peak shape. Resolving power is inversely proportional to mass in FTICR, so it is important to know the mass at which a given resolving power was obtained in order to determine what the resolution should be at another mass. Time-of-flight mass spectrometers also usually use the 50% peak-height definition. Peak shapes in time-of-flight are Gaussian.

Consider the difference between the definition of unit resolution and resolving power as defined in a magnetic sector mass spectrometer. If we have **5000 resolving power** on a magnetic sector mass spectrometer, we can separate m/z 50.000 from m/z 50.010, or separate m/z 100.000 from m/z 100.020, or separate m/z 1000.000 from m/z 1000.200 (all down to a 10% valley between the two peaks). **Unit resolution** would allow you to distinguish m/z 50 from m/z 51, or distinguish m/z 100 from m/z 101, or distinguish m/z 1000 from m/z 1001.