Intro to MS Resolution & Accuracy

CU- Boulder

CHEM-5181

Mass Spectrometry & Chromatography

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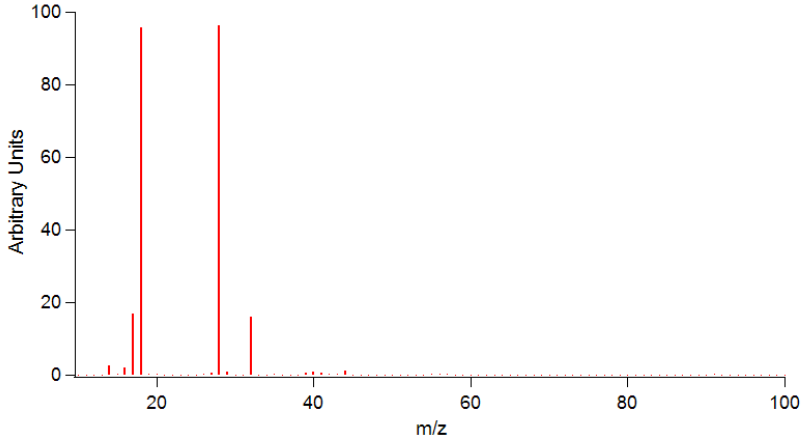
Some slides adapted from 2007 lecture by Dr. Joel Kimmel, CU-Boulder

Mass Spectrum



Signal intensity vs mass-to-charge ratio

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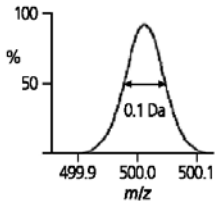
Mass Analyzer Resolving Power

Figure 1: Mass accuracy determination and the FWHM method for determining resolution for a mass spectrometer measured at a given ion.



True mass = 400.0000
Measured mass = 400.0020
Difference = 0.0020 or 2 mmu
Error = $\frac{0.002}{400} \times 10^6 = 5$ ppm

Mass = 500
Peak width (@ 50%) = 0.1
Resolution (FWHM) $\frac{500}{0.1} = 5000$

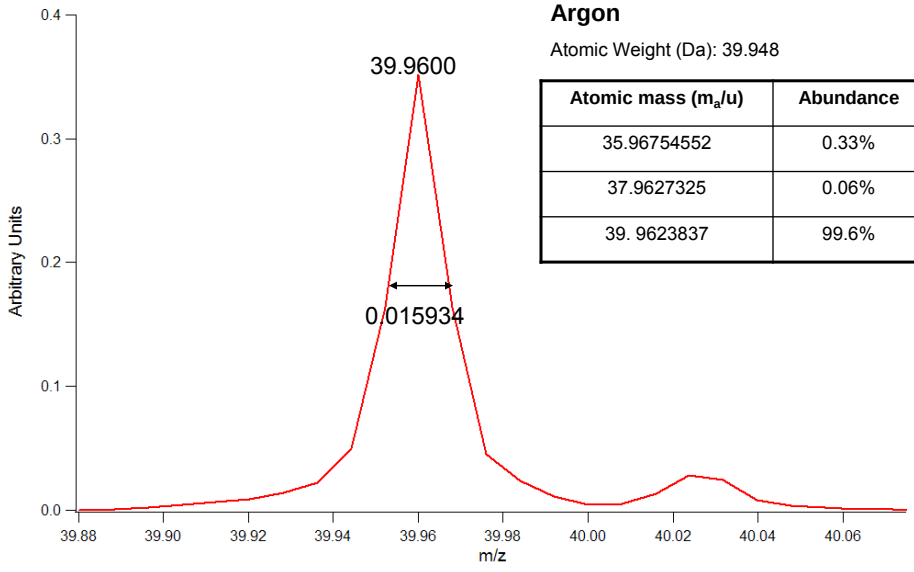
Mass peak width ($\Delta m_{50\%}$)
Full width of mass spectral peak at half-maximum peak height

Mass resolution / Resolving Power (m / $\Delta m_{50\%}$)
Quantifies ability to isolated single mass spectral peak

Mass accuracy
Mass accuracy is the difference between measured and actual mass

Figure from: M. P. Balogh, *LC-GC Europe*, 17(3), 152–159 (2004) 3

Calculate resolution and accuracy



Argon

Atomic Weight (Da): 39.948

Atomic mass (m_a/u)	Abundance
35.96754552	0.33%
37.9627325	0.06%
39. 9623837	99.6%

N

Mass Analyzer Resolution II

- Question: what is the resolution (FWHM definition) in both cases
  - if m_1 = 50 Da?
  - If m_1 = 2500 Da?

  ($m_2 = m_1 + 1$ amu)

From Hoffmann

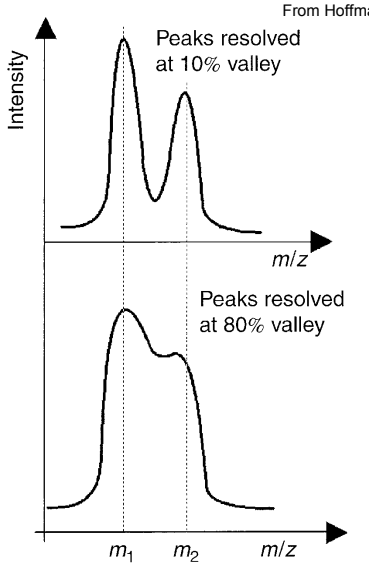


Figure 2.1
Diagram showing the concepts of peak resolution and valley

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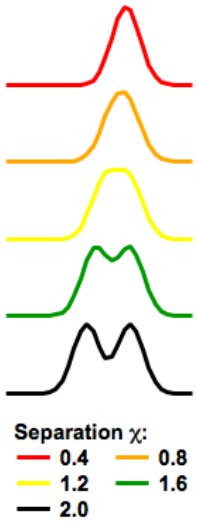
What Resolution do we really need?

- What resolution is really needed to distinguish these two overlapping ions, *if we know that only these two ions are present*?
  - A. χ = 0.4
  - B. χ = 0.8
  - C. χ = 1.2
  - D. χ = 1.6
  - E. χ = 2.0



χ = peak separation / HWHM

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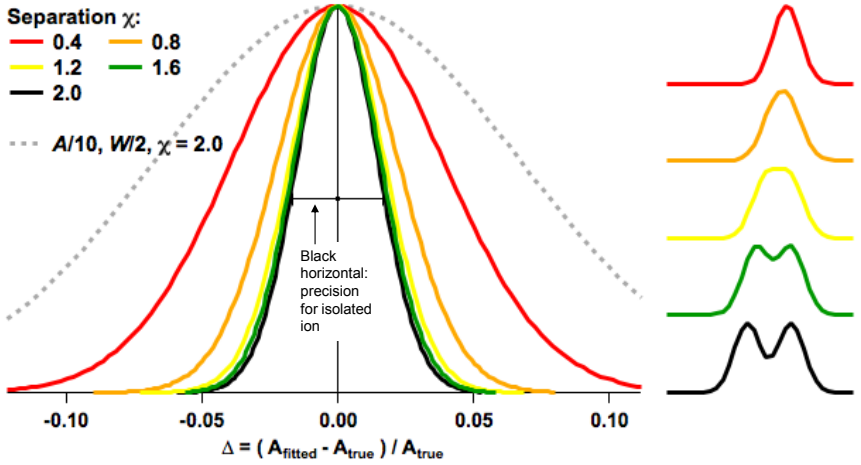
What Resolution do you really need?



χ = peak separation / HWHM

Cubison and Jimenez, 2013 in prep.

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Clicker Q: A mass spectrometer with a resolution of 5000 should be capable of resolving isotopic peaks (e.g. $^{12}CH_4$ vs $^{13}CH_4$) for singly charged species with *m/z:*

(a) Of any value
(b) Less than *m/z* 5000
(c) Greater than *m/z* 5000
(d) It depends on the type of mass spectrometer
(e) I don't know

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