KORE TECHNOLOGY

Mass Resolution of Kore PTR-TOF-MS, Series II Instrument 2013

Kore Technology Ltd. has developed a high mass resolution TOF spectrometer that is now fitted to the PTR-TOF-MS Series II instruments.

When fitted to a PTR-TOF-MS, the spectrometer routinely delivers a mass resolution performance of >5,000 (FWHM) at low mass and at full transmission. Sensitivity can also be traded off against mass resolution, and this spectrometer has produced up to 10,000 (FWHM) at low mass.

Reporting Mass Resolution

Raw data vs. Gaussian fitting

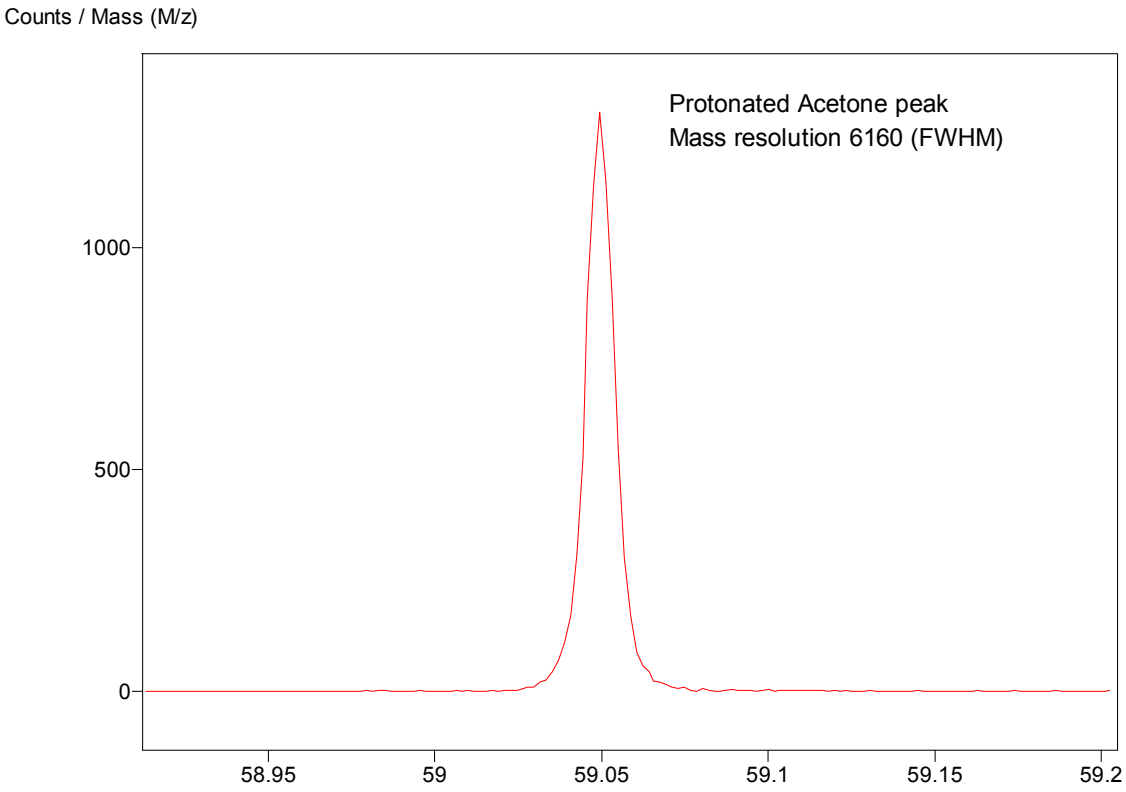
Ways of reporting mass resolution can vary. Clients should be aware of this when comparing statements of mass resolution. In the data below, Kore shows 'untreated' data and reports resolution based on the 'raw' data. This is time data converted directly to mass. The mass peaks in the Kore PTR instrument are not symmetrical (there is no reason why they should be in a TOF), but they are often close to a Gaussian, apart from a slight tail usually on the high mass side (depends on reflectron tuning). We do not employ curve fitting to 'extract' a gaussian peak which then becomes the basis for a mass resolution measurement. This latter method serves to increase the reported mass resolution, but is artificial (see example at end of document). This is why we always show the raw data and reported mass resolution based on that data. Peak fitting and deconvolution is legitimate when attempting to extract peak integrals from peaks with significant overlaps. This is a well-proven method in a quantitative technique such a x-ray photoelectron spectroscopy (xps)

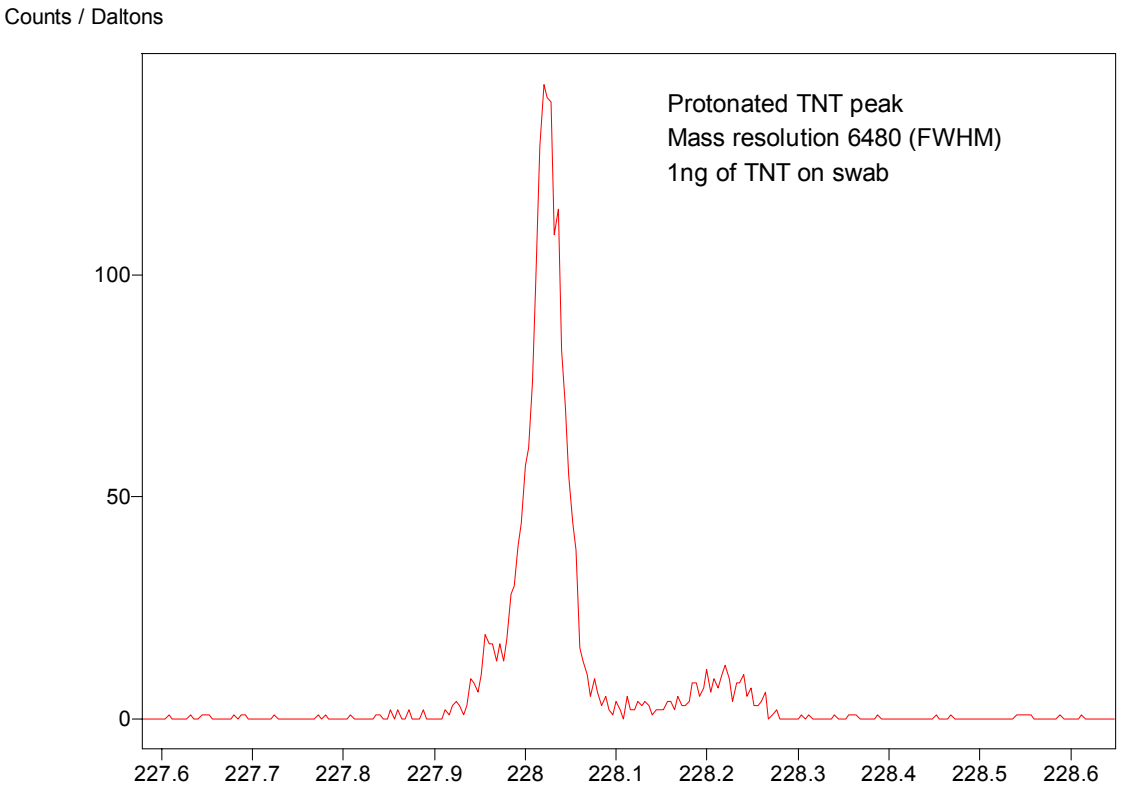
In the Kore instrument the software 'finds' peaks according to user defined criteria (peak area, smoothing points etc) and determines the height of the peak with reference to an adjacent baseline. In most cases that baseline is at or very near to zero because the PTR-TOF-MS does not have a Bremsstrahlung-type background. The software calculates the half height of the peak and then finds the equivalent width in mass units. The resolution is then the absolute mass value of the peak divided by the mass width of the peak at half height, and is reported by the software

Split peaks

In the case of a split peak where the peaks are not separated down to the baseline, it is not legitimate to define the peak height as that distance from the top of the peak down to where it meets the adjoining peak. The height must be defined from the baseline to the top of the peak.

Examples of PTR-TOF-MS mass resolution at full transmission





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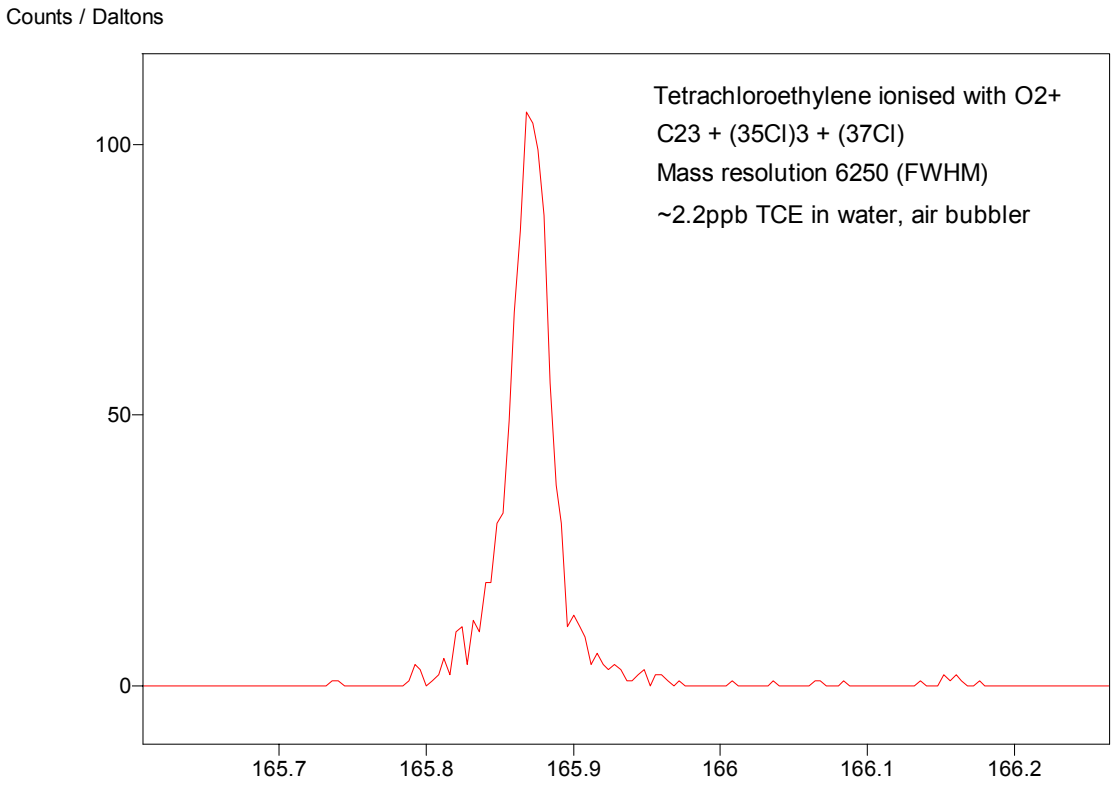
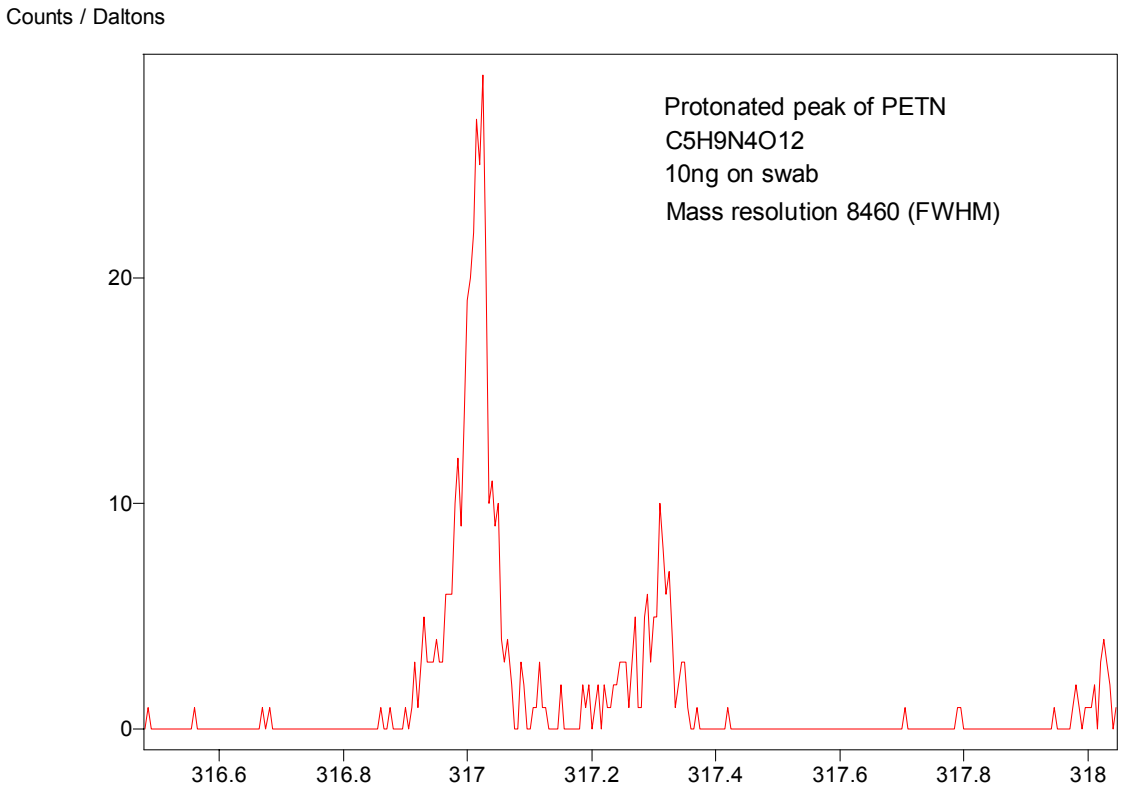
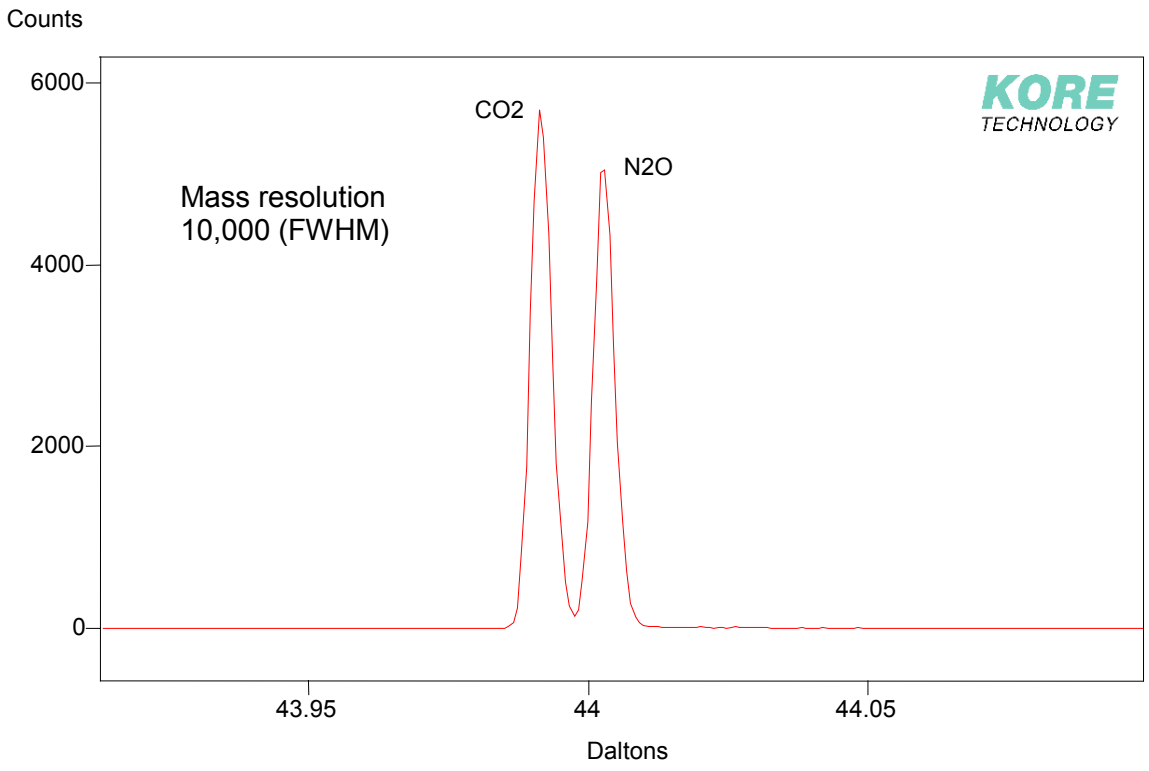


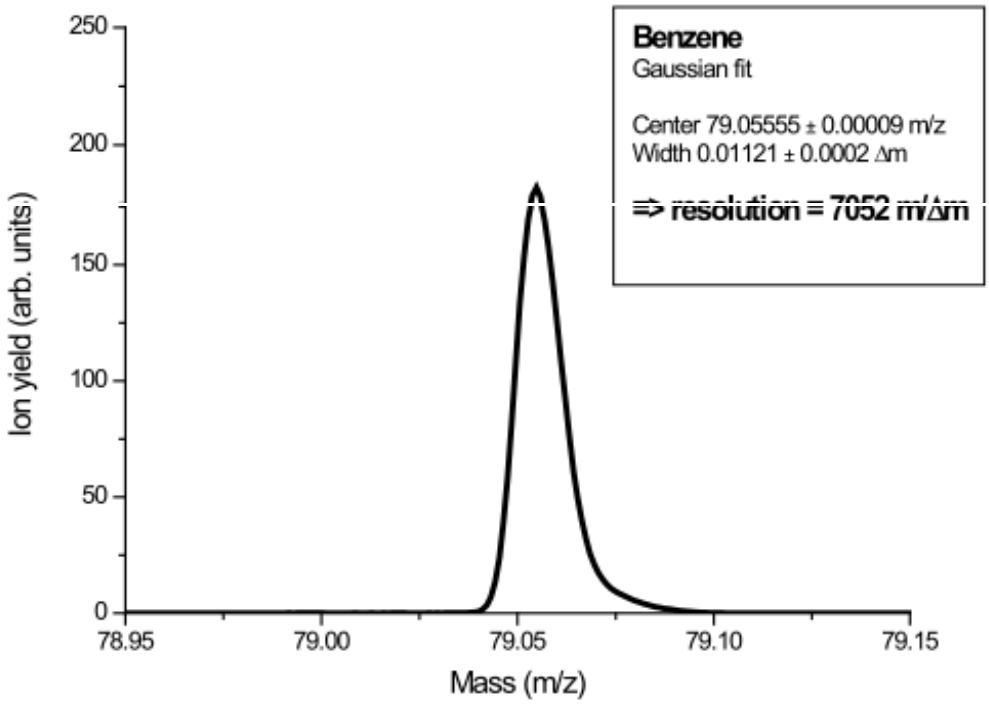


Example of high mass resolution at reduced transmission (aperture)



Data obtained from the new TOF spectrometer, showing baseline separation of CO_2 and N_2O at mass 44. Mass resolution 10,000 (FWHM). This data was taken using an electron impact ion source and an instrument with an aperture at a focal point in the ion optics. This reduces the transmission but increases the mass resolution.

Example of different method of reporting mass resolution



In the above example, a peak is shown for benzene. The information box quotes a mass resolution value of 7,052 using a 'Gaussian fit' (curve not shown). However, if one measures the full width at half maximum of the actual peak (and not a mathematically generated curve), it measures somewhere between 5,600 and 5,750 and is not 7,052.

Care must be taken when reporting and comparing values of mass resolution.