Using Van Krevelen Plots To Determine Molecular Formulae From Exact Masses

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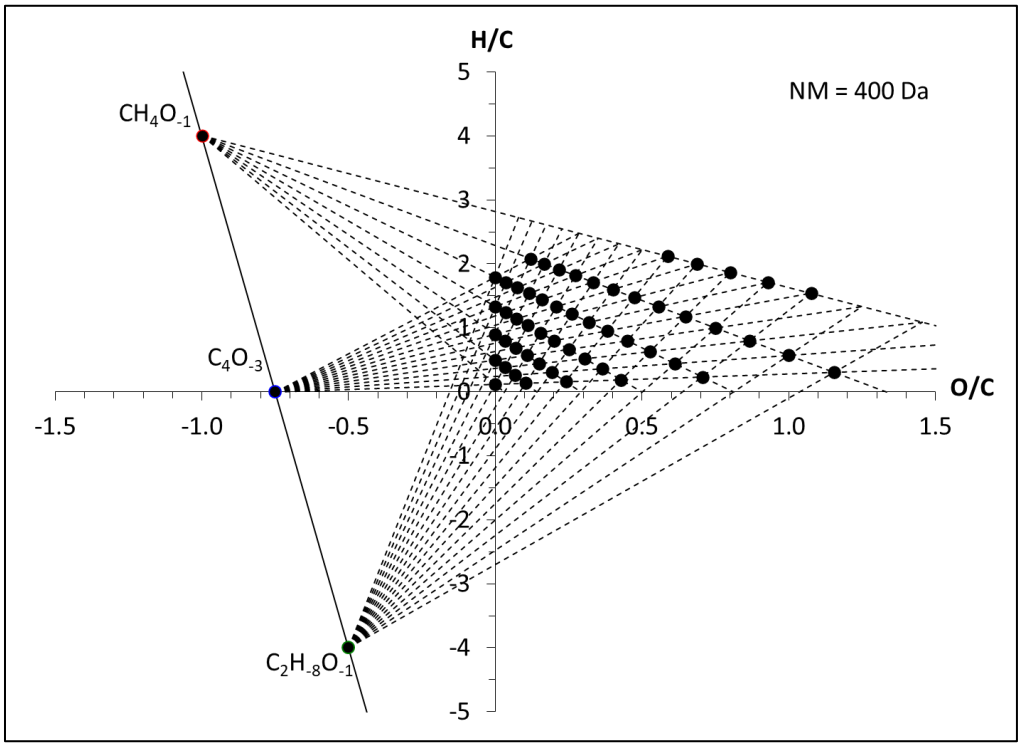
In the interpretation of ultra-high resolution mass spectra, very small mass differences are often attributed to "substitutions" such as the replacement of CH_4 by O. Perdue and Green (**Anal. Chem., 2015, 87, 5079−5085**) proposed that such mass pairs should be written as molecular formulae (CH_4O_{-1}), with corresponding nominal masses (NM) and exact masses (EM). They introduced the term of low-mass moieties (LMM's). This particular LMM has NM=0 and EM=+0.0363855 Da.

Perdue and Green also demonstrated that a Van Krevelen plot of all valid isobaric molecular formulae for molecules composed of C, H, and O displays several series of non-parallel lines that intersect at specific locations in negative quadrants of Van Krevelen space. Here is Figure 3 from their paper.



This lecture will demonstrate how the information in Figure 3 can be used to ***rapidly*** determine the molecular formula of a molecule from its exact mass. Extension of the algorithm to molecules containing N, S, P, and ^{13}C is straightforward, and computer codes based on this algorithm are significantly faster than all other tested computer codes. The current version of CHOFIT3 requires only one second to assign molecular formulae to 21268 mass peaks in an FTICR mass spectrum of Suwannee River NOM.
