

### Predicting MS Spectra

The analysis of MS spectra is merely the reversal of the prediction of spectra. Knowing the possibilities is key to the interpretation of spectra. Always consider the isotopic peaks and the fragmentation pattern.

(a) 2-Mercaptobenzoic acid

(b) Consider the relative abundances of the (M-H) and (M-Me) peaks in the 70eV EI MS spectra of 2-methylpyrrole and 2-acetylpyrrole.

(c) Predict the spectrum of diphenyl ether. There also is a not-so-expected peak with  $m/z=142$  resulting from CO loss. Give a mechanism for the formation of this ion.

(d) Predict the fragmentation reactions for leucine,  $\text{H}_7\text{C}_3\text{-CH}_2\text{-CH(NH}_2\text{)-COOH}$ .

(e) Predict the EI and CI ( $\text{H}^+$ ) spectra of 4-methylbenzophenone.