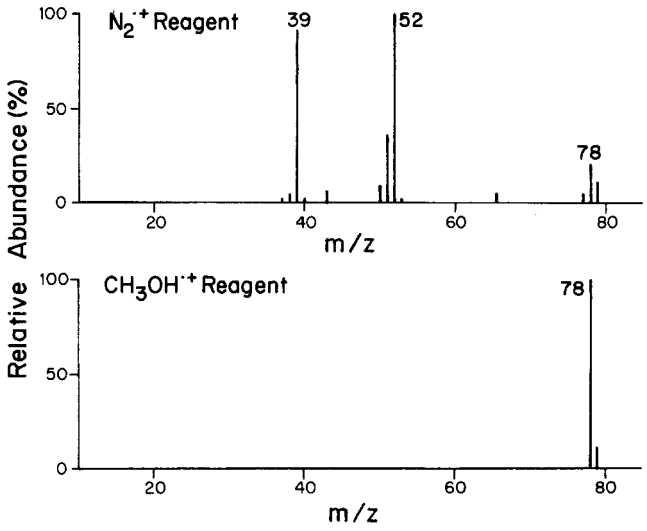
Chemistry 416, Dr. Glaser

Applications of Mass Spectropscopy: Chemical Ionization of Benzene.

Chemical Ionization of Benzene

The spectra are shown of benzene after chemical ionization with the reagent gases $CH_3OH^{\bullet+}$ and $N_2^{\bullet+}$. In one case, the molecular ion is abundant while fragmentation has occurred in the other.



The degree of fragmentation depends on the energy transferred onto the sample molecules at the time of ionization. This energy does depend on the difference between the ionization energies for the sample and the reagent gas. Determine the maximum amount of energy that can be transferred to benzene from the two reagent gases. The ionization energies of benzene, methanol, and dinitrogen are 9.25, 10.85, and 15.6 eV. Do your calculations in electronvolts and then also give the final numbers in kcal/mol. Discuss the resulting numbers under consideration of typical bond dissociation energies. Suggest a fragmentation path for benzene that explains the fragment ions seen in the top spectrum.

(1 atomic unit = 27.211 eV = 627.51 kcal/mol)