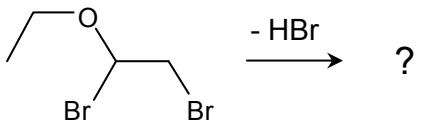
Chemistry 2301

Workshop 24
Structure Determination with NMR

Morgan, a chemist, had planned to use 1,2-dibromo-1-ethoxyethane (drawn below) as a starting material in a substitution reaction. However, he found that even weak Lewis bases caused the molecule to decompose before it could react as intended. He isolated two decomposition products with identical molecular formulae C_4H_7BrO;[1] because the starting material has formula $C_4H_8Br_2O$, Morgan concluded that both products were generated by elimination of HBr.

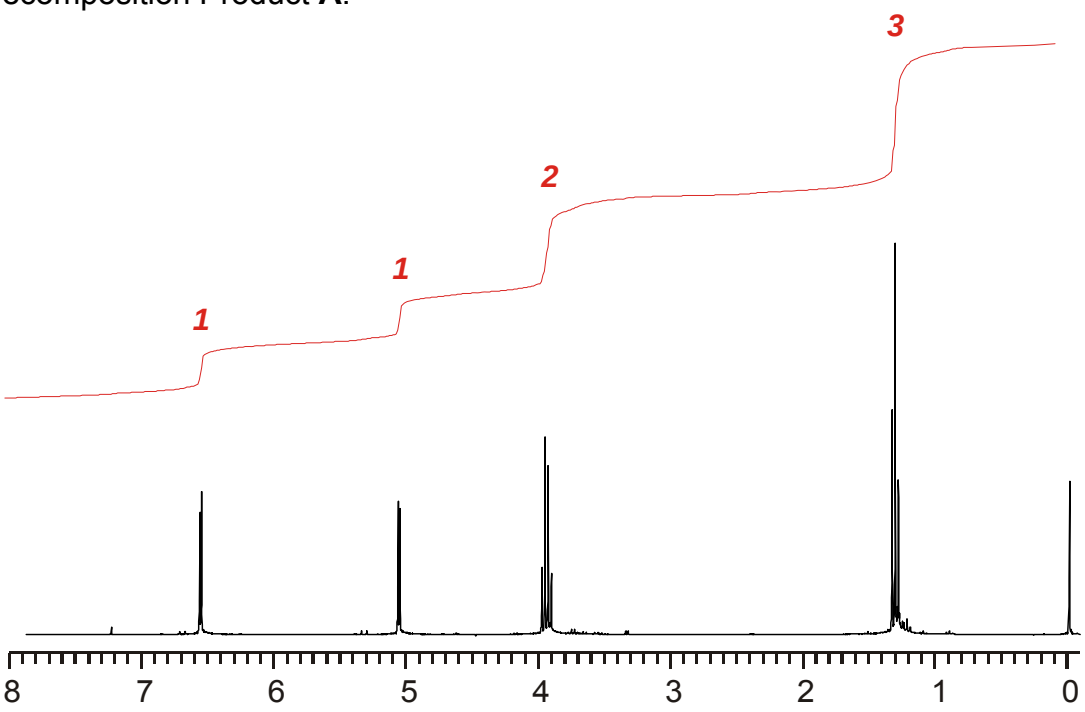


Use the NMR spectra of the two decomposition products, shown on the following two pages, to determine the structures of the two molecules. Use what you know—not only about the chemical shifts and coupling constants in the molecule, but also about the starting material and reaction—to test hypotheses about which product structure might correspond to each product spectrum.

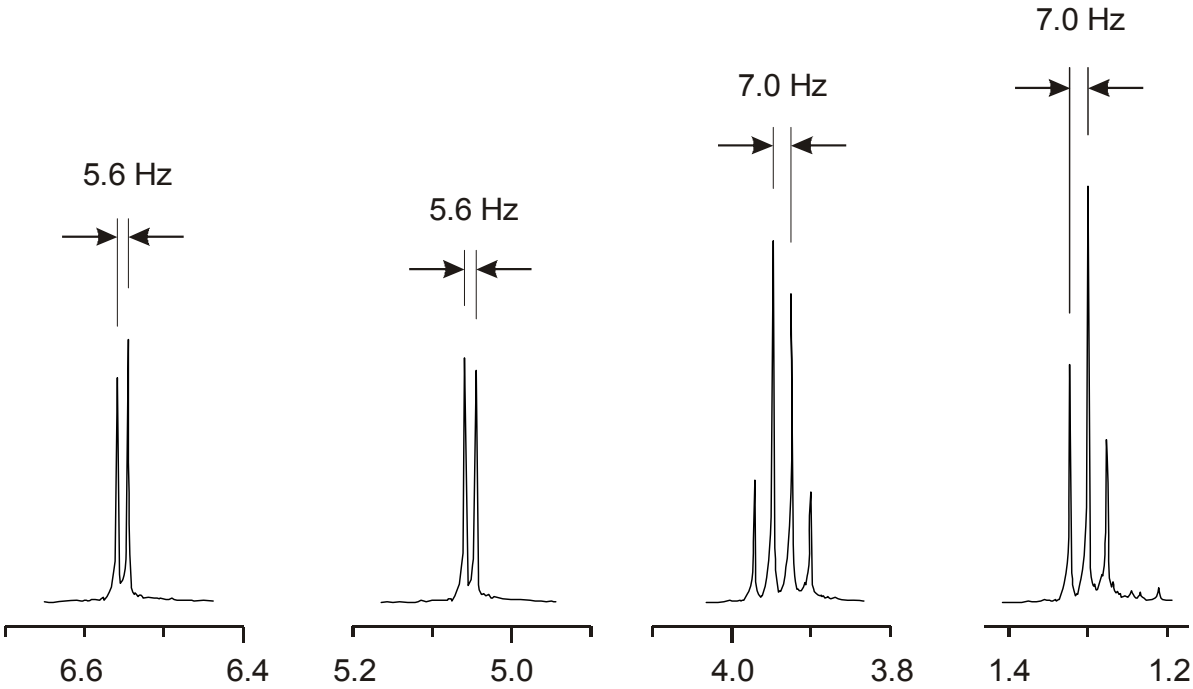
Note: Coupling constants *J* (in Hz) have been calculated for you in this problem—there is no need to determine $\Delta\delta$ (ppm) and then convert these to Hz.

[1] Morgan obtained these molecular formulae by high-resolution mass spectrometry, which you will learn about in Chapter 12.

Decomposition Product **A**:



^{1}H NMR, 300 MHz



Decomposition Product **B**: