Report Instructions Preparation and Analysis of an Ester of Phosphorous Acid

Percent Yield

Calculate the percent yield of Compound B, assuming that 1.1 g of Product A was used.

Infrared Analysis

On the spectra themselves, identify bands that correspond to the following types of stretching vibrations: C-H, N-H, P-H, P=O. (Some spectra will not contain some of these absorptions.)

NMR Analysis

Make all of the NMR assignments directly on printouts of the spectra.

- 1. Assign all ¹H NMR signals that correspond to products A, B, C, and D. For Product C, you need only identify the signals from Product C; the impurity signals can be ignored.
- 2. Assign all ¹³C NMR signals that correspond to products A, B, and C. For Product C, you need only identify the signals from Product C; the impurity signals can be ignored. Aromatic signals should be assigned as a group, since it is difficult to make the individual assignments with certainty.
- 3. Identify all coupling constants of ³¹P with ¹H and with ¹³C. These can be indicated on either the ³¹P or ¹H spectra. Any ³¹P/¹³C coupling constants must be assigned using the ¹³C spectra.

The values for the coupling constants can be calculated from the line lists that are provided with some of the NMR spectra. They should be reported in Hertz (Hz, frequency units), rounded to the nearest Hz.

Report the values as ${}^{n}J_{AB}$, where n is the number of bonds between the coupled atoms, and AB describes the coupled atoms (for example, PH).

Draw a horizontal line between the peaks that you use for your coupling constant calculations, and indicate the coupling to which it refers.

4. Draw the structure of the product on each spectrum that you turn in.

Extra Credit

Provide reasonable mechanisms for the formation of Products A, B, C, and D. Keep in mind that a fifth, gaseous, organic product is produced in the first reaction along with Product A. Its ¹H NMR spectrum consists of a singlet at 3.05 ppm.