Convergent Multi-Step Synthesis of Hexaphenylbenzene

Background Information:

In this experiment you will synthesize hexaphenylbenzene via a 7-step, convergent synthetic pathway. Organic synthetic pathways can be linear or convergent. In a linear synthesis, as shown in figure 1 below, a single linear sequence of synthetic steps affords the product of interest. On the other hand, a convergent synthetic scheme is made of two or more linear sequences that are eventually combined (converge) to afford the final synthetic target.

**Linear Synthesis**

\[
\begin{array}{c}
A \\ B \\ C \\ D (\text{final synthetic target})
\end{array}
\]

**Convergent Synthesis**

\[
\begin{array}{c}
A \\ B \\ C \\ F (\text{final synthetic target}) \\
D \\ E
\end{array}
\]

**Figure 1. A general depiction of linear and convergent synthetic pathways.**

Fluency in carrying out organic laboratory techniques, preparation, and organization will enhance the success and efficiency of your experiment, which will show in the Overall Percent Yield. In addition to percent yield calculations for individual steps, the overall percent yield should be calculated and reported. The overall percent yield is the product of all the individual percent yields. For example, if in a four-step synthesis, the individual yields are calculated to be 80%, 90%, 95%, and 70%, the overall percent yield is equal to:

\[
\frac{80 \times 90 \times 95 \times 70}{100 \times 100 \times 100} = \frac{4,788,000}{100,000,000} = 48\%
\]

As seen, minor losses in individual steps end up resulting in substantial diminishing of the overall % yield.

Hexaphenylbenzene, your synthetic target, is a highly symmetric hydrocarbon, with a melting point of 465°C. This is an unusually high melting point for organic compounds. Figure 2 below, shows the structure for this compound.

**Figure 2. Lewis structure for hexaphenylbenzene.**
Overview of the synthetic pathway:

Figure 3. Convergent synthetic scheme for hexaphenylbenzene.
As seen in Figure 3 above, two linear branches, each starting with benzaldehyde and going through 3 steps, merge to form the final product of interest.