Problem Set #6
Solutions

1. a) \( \text{NaI} \rightarrow \)
   
   Some other leaving group is OK

b) \( \rightarrow \)

c) \( \text{NaN} \rightarrow \)

d) \( \rightarrow \)

Note: In these problems there’s flexibility regarding choice of leaving group and solvent
\( \text{H}_3\text{C} - \text{N} - \text{C}l \)

Regular 1° alkyl halide

No SN1

\[
\text{H}_3\text{C} - \text{N} - \text{C}l \quad \text{slow} \quad \text{H}_3\text{C} - \text{O} - \text{C}l
\]

Normally, a 1° carbocation would require a prohibitive amount of activation energy to form.

But, this cation is RESONANCE-STABILIZED:

all atoms have full octets.
The $t$ for form of this carbocation looks a lot like carbocation, and is similarly stabilized.

\[
\begin{align*}
\text{best e.g.} & \quad \text{(weakest base)} \\
\text{Conjugate acids} \\
\text{strong acid}
\end{align*}
\]
(R)-2-bromooctane

\[ \xrightarrow{\text{H}_2\text{O}/\text{EtOH}\#} \]
expect mainly SN 1
w/ maybe some SN 2

(R)-2-octanol
Product of substn
with retention of configuration

(S)-2-octanol
Product of substn with inversion

(R)-2-octanol is known to have a negative rotation (this was given in the problem), so the major product of the above run must be the (S) enantiomer for a positive optical
rotation to be observed. This means the reaction proceeds with an excess of inversion over retention.

\[ \text{H}_2\text{O} \quad \text{vs} \quad \text{Na}^+ \quad \text{\text{ OH} \quad \boxed{\text{better nucleophile}} } \]

\[ \text{H}_3\text{N} \quad \text{vs} \quad \text{K}^+ \quad \text{\text{ N-H} \quad \boxed{\text{better nucleophile}} } \]

\[ \text{Na}^+ \quad \text{\text{ S-CH}_3 \quad \boxed{\text{better nucleophile}} } \]

\[ \text{H} \quad \text{\text{S-CH}_3 \quad \boxed{\text{better nucleophile}} } \]

\[ \text{H}_3\text{C} \quad \text{\text{O} \quad \boxed{\text{better nucleophile}} } \]

\[ \text{F}_3\text{C} \quad \text{\text{O} \quad \boxed{\text{better nucleophile}} } \]

\[ \text{we change stabilize by electron withdrawing F's. Less nucleophilic} \]
Double inversion leads to overall retention.

Inversion #1

Inversion #2

Product