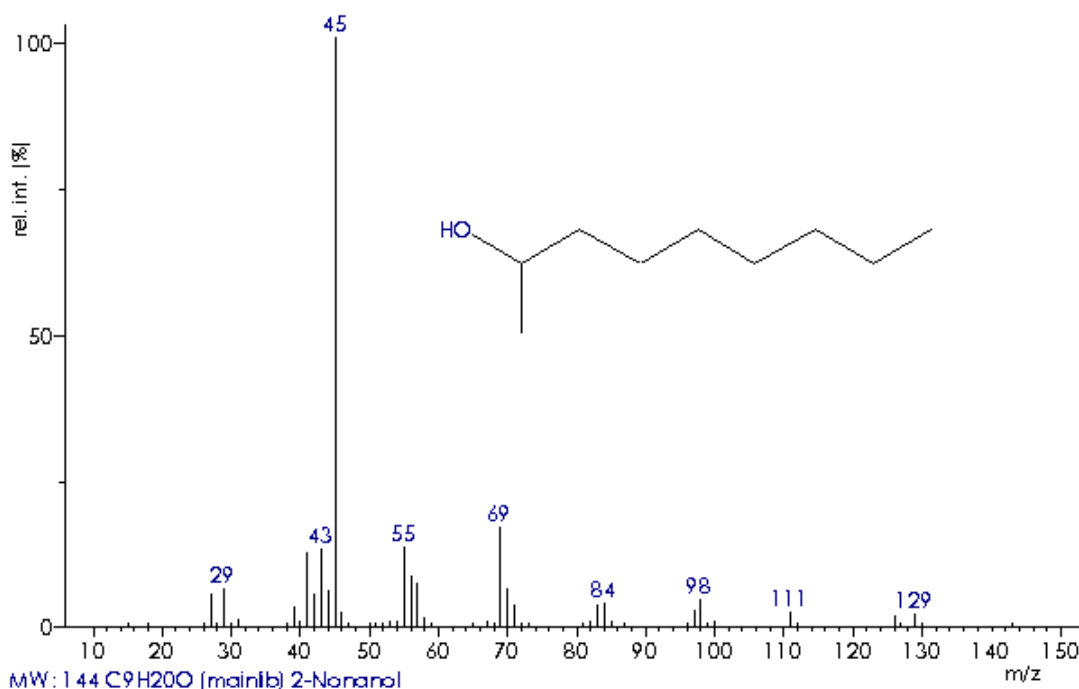


## Answer 6.17

Identify the unknown from its 70 eV EI mass spectrum.

The positive-ion CI mass spectrum, isobutane reagent gas, showed a strong signal at  $m/z$  143 and a weaker signal at  $m/z$  145.

The presence of halogens can be excluded from the synthetic pathway.



The highest-mass ion in the EI mass spectrum is found at  $m/z$  143, but it gives neutral losses of 14 u to the next lower  $m/z$  peak. However, if  $m/z$  129 was  $[\text{M}-\text{CH}_3]^+$  we had  $M = 144$  u, and then, its companion at  $m/z$  126 could be explained as  $[\text{M}-\text{H}_2\text{O}]^+$ , i.e., the EI spectrum doesn't exhibit a molecular ion peak. Together with  $m/z$  98,  $[\text{M}-18-28]^+$  and the base peak at  $m/z$  45 (oxonium ion!?) these findings point towards an aliphatic alcohol.

**CI:** Aliphatic alcohols yield no or weak  $[\text{M}+\text{H}]^+$  ions in CI, but hydride abstraction forms dominant  $[\text{M}-\text{H}]^+$  ions. This agrees with the observation and the assumptions made in the preceding paragraph.

Thus, we have  $M = 144$  u and even mass indicates 0, 2, 4, ... nitrogen atoms.

→ Unknown contains  $\geq 1$  oxygen atom(s) and alcohol or ether group(s).

Try first with a simple alcohol: empirical formula:  $C_9H_{20}O$ ;  $r+d = 9 - 10 + 1 = 0$

Fragmentation scheme:

