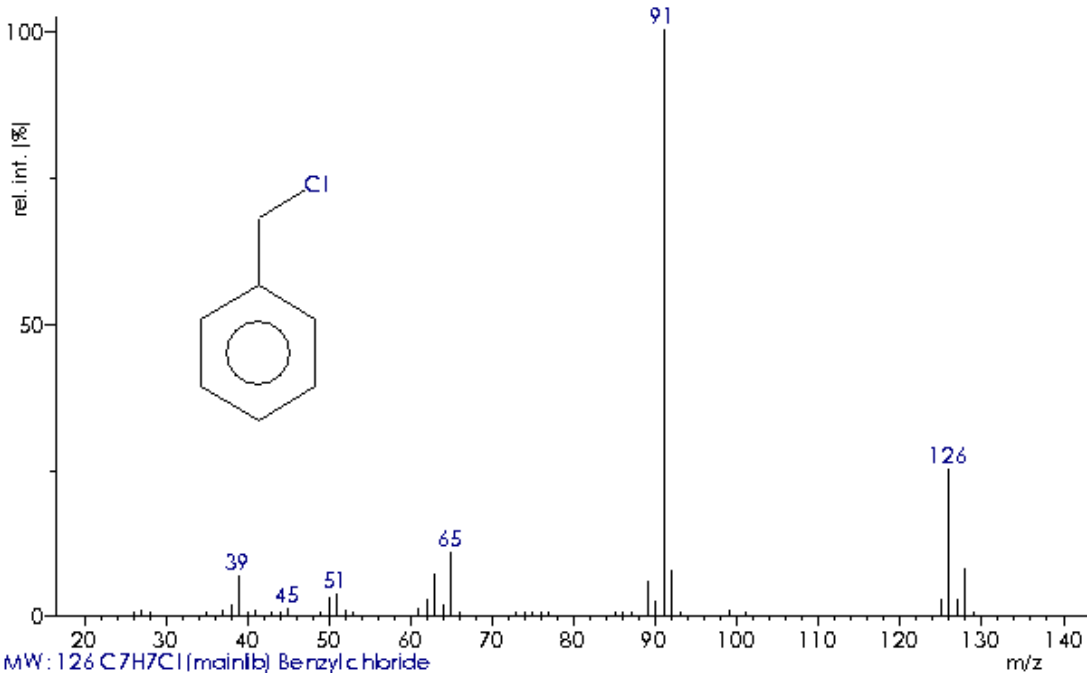
Answer 6.9

Identify the unknown from its 70 eV EI mass spectrum.



The (presumed) monoisotopic molecular ion peak is of medium intensity (→ aromatic rather than aliphatic compound), located at *m/z* 126, and exhibits a Cl isotopic pattern (126, 128). Again, even mass indicates that the molecule contains 0, 2, 4, ... nitrogen atoms.

The ^{13}C peak has 11 % of *m/z* 126 (use a ruler), i.e., one expects roughly 10 carbon atoms. As there is a $[M–H]^+$ peak, *m/z* 125, the carbon number will be overestimated due to the fact that the ^{13}C peak of the „^{35}Cl ion“ and the $[M–H]^+$ peak of the „^{37}Cl ion“ are also isobars.

m/z 91 (base peak)	[M–35], no Cl pattern → $[M–Cl]^+$
m/z 65	[M–35–26] → loss of C_2H_2 from $C_7H_7^+$?
m/z 51	
m/z 39	→ series 39, 51, 65, 77 (weak), 91 perfectly fits behavior of $C_7H_7^+$ ions

The sum of 91 u + 35 u explains the molecular ion peak.
Now, the molecular formula C_7H_7Cl can be expected; r+d = 7 – 0.5 × (7 + 1) + 1 = 4

We have either benzylchloride or some chlorotoluene isomer. Benzylchloride is slightly preferred, because doubly substituted aromatic systems show the series *m/z* 39, 51, 65, 77 more diffuse and typically shifted by 1 u to lower mass.

Fragmentation scheme: