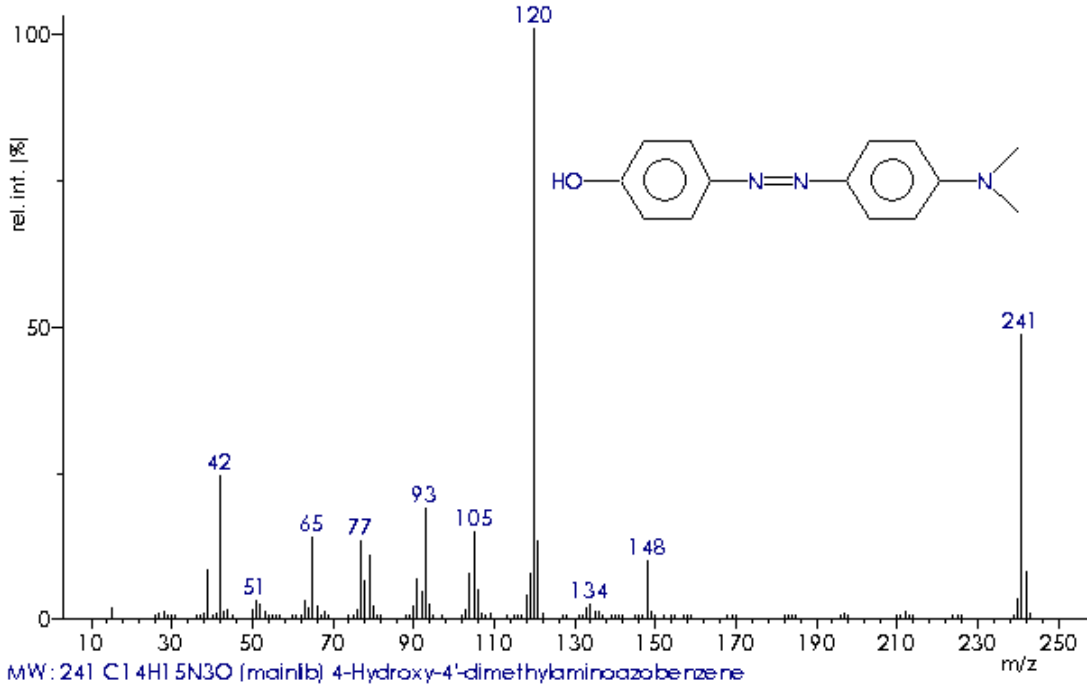
Answer 6.18

Identify the unknown from its 70 eV EI mass spectrum.
The compound has a deep orange color.
HR-MS: *m/z* 241.1220, *m/z* 148.0855, *m/z* 120.0800.



The molecular ion, $M^{+\bullet}$ = 241, is very stable.
Its odd mass indicates 1, 3, 5, ... nitrogen atoms.
The isotopic pattern shows no Cl, Br, Si or S.
From the ^{13}C-peak (17 %, use a ruler) we estimate 14–16 carbons.
The intensity distribution points towards an aromatic or heterocyclic compound.

m/z 148	[M–93]
m/z 120	[M–121]
m/z 105	benzoyl ion?
m/z 93	[M–148], phenolic?
m/z 77	$[C_6H_5]^+$?

The ions/losses 148, 93 and 120, 121 form pairs with total mass equal to *M*.

HR-MS: Exploit the differences between accurate *m/z* values to identify neutral losses.
i) 241.1220 u – 148.0855 u = 93.0365 u which fits $[C_6H_5O]^+$ (calc. 93.0335 u) as can be expected for phenolic sub-structure;
ii) 241.1220 u – 120.0800 u = 121.0420 u, no idea at first sight.

Color presents the key to solve this problem. Assume an azodye; add the mass of N_2: 93.0365 u + 28.0061 u = 121.0396 u correlating well with neutral loss of $C_6H_5ON_2$ (calc. 121.0402 u).

Now, at least 3 nitrogen atoms are required to explain the odd mass of $M^{+\bullet}$.

Try to fill the remaining 120 u with C, H, and 1 N. The formula $[C_8H_{10}N]^+$ (calc. *m/z* 120.0808) fulfils these criteria.

Molecular formula: $C_{14}H_{15}N_3O$; exp. *m/z* 241.1220, calc. 241.1210, o.k.
r+d = 14 – 7.5 + 1.5 + 1 = 9

Fragmentation scheme: