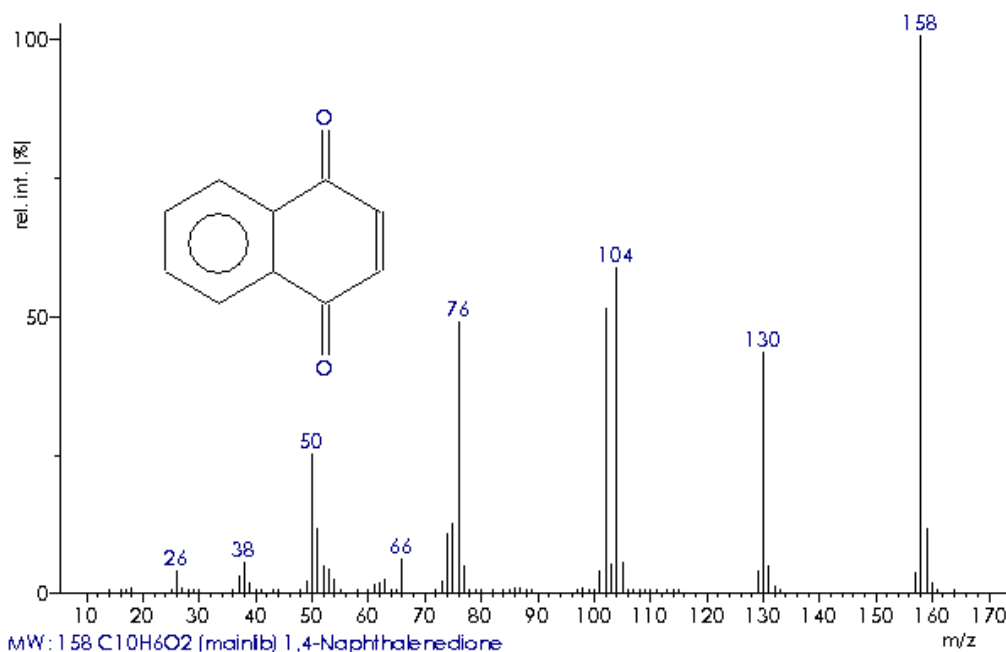


Answer 6.13

Identify the unknown from its 70 eV EI mass spectrum. From an accurate mass measurement, neutral losses of 26 u could be assigned to C₂H₂ while neutral losses of 28 u correspond to CO.



Loss of C₂H₂ frequently occurs from aromatic systems or from quinones. CO loss is common to phenols, quinones, and many other carbonyl compounds. Both fragmentations are observed in case of phenols or quinones.

The molecular ion, M⁺ = 158 (base peak), is very stable and its even mass indicates 0, 2, 4, ... nitrogen atoms.

The isotopic pattern shows no Cl, Br, Si or S.

From the ¹³C-peak (11.5 %, use a ruler) we estimate 10–11 carbon atoms.

m/z 130	[M–28], [M–CO] ⁺
m/z 104	[M–28–26], [M–CO–C ₂ H ₂] ⁺
m/z 102	[M–28–28], [M–CO–CO] ⁺
m/z 76	[M–28–28–26] or [M–28–26–28], i.e., [M–CO–CO–C ₂ H ₂] ⁺ or [M–CO–C ₂ H ₂ –CO] ⁺
m/z 50	[M–(CO) ₂ –(C ₂ H ₂) ₂] ⁺ , aromatic fragment „–1 u“
m/z 38	aromatic fragment „–1 u“
m/z 26	C ₂ H ₂ ⁺

A maximum loss of two CO molecules coincides with a quinone.

Subtracting the mass of two CO (2×28 u) and two acetylene molecules (2×26 u) from 158 u leaves 50 u \rightarrow C₄H₂?

The molecular formula is C₁₀H₆O₂; $r+d = 10 - 3 + 1 = 8$

The $r+d$ of an aromatic ring is 4, another 2 are for the carbonyls and another 2 for the second ring with one double bond.

Fragmentation scheme:

