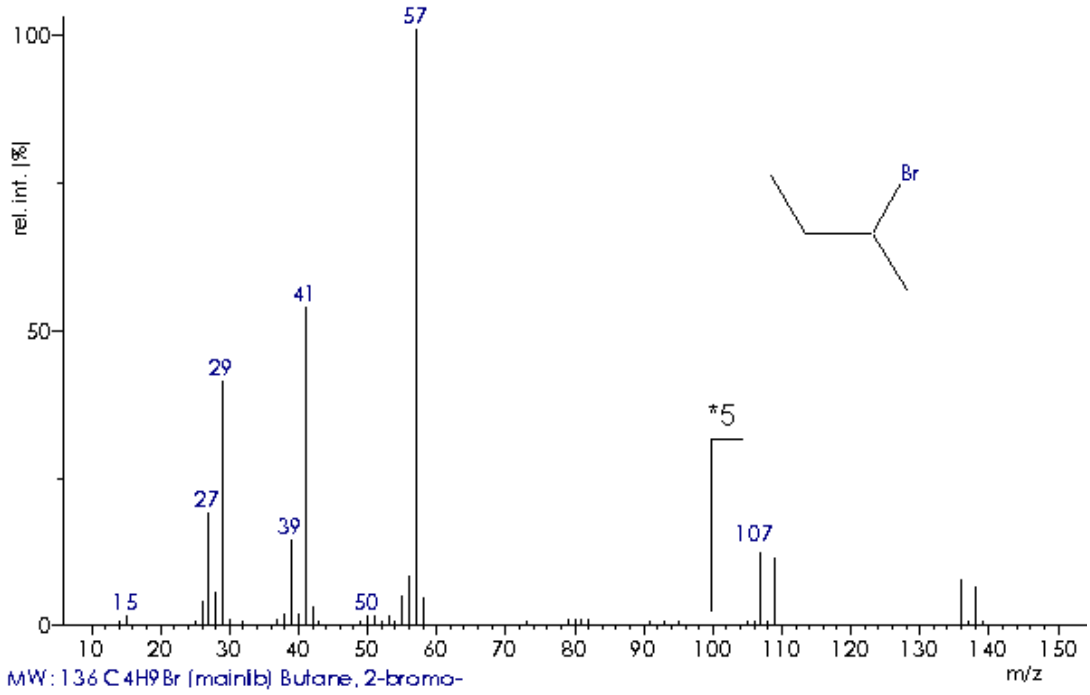
Answer 6.8

Identify the unknown from its 70 eV EI mass spectrum.



Starting from *m/z* 100, the intensities are shown magnified fivefold.
Crawl across the mass spectrum to identify typical isotopic patterns, obvious mass differences, i.e., neutral losses, and/or well-known fragment ions or fragment ion series:

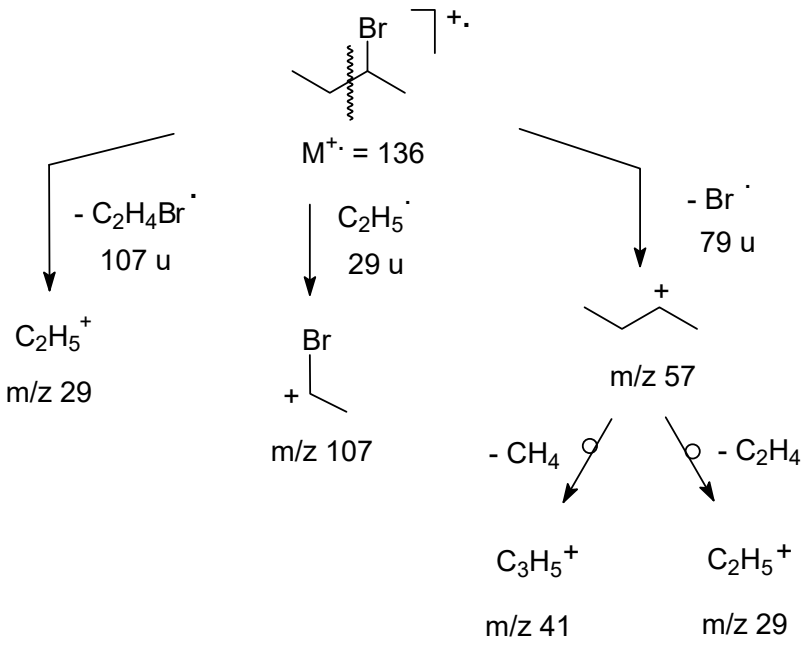
The monoisotopic molecular ion peak is weak, located at *m/z* 136 (most probably), and exhibits a Br isotopic pattern (136, 138). Even-numbered mass indicates 0, 2, 4, ... nitrogen atoms.
^{13}C peaks are small, i.e., there are few carbons.

m/z 107, 109 (weak)	Br pattern, $[M–29] \rightarrow [M–C_2H_5]^+$
m/z 80, 82 (weak)	Br pattern $\rightarrow HBr^{+\bullet}$
m/z 79, 81 (weak)	Br pattern $\rightarrow [M–57] \rightarrow [M–C_4H_9]^+ \equiv Br^+$
m/z 57	$[M–79] \rightarrow [M–Br]^+$
m/z 39, 41	
m/z 27, 29	$\rightarrow$ series 27, 29, 39, 41, 57 perfectly fits the behavior of butyl ions

As we have one bromine, the remaining mass of the unknown is 136 u – 79 u = 57 u which should correspond to C_4H_9.
Thus, the empirical formula is C_4H_9Br; r+d = 4 – 0.5 × (9 + 1) +1 = 0

Here, the EI mass spectrum alone does not perfectly identify the isomer. However, the preferred loss of ethyl as compared to methyl or propyl indicates 2-bromobutane. One should compare the spectrum with reference spectra of the isomers.

Fragmentation scheme:



only monoisotopic masses are shown