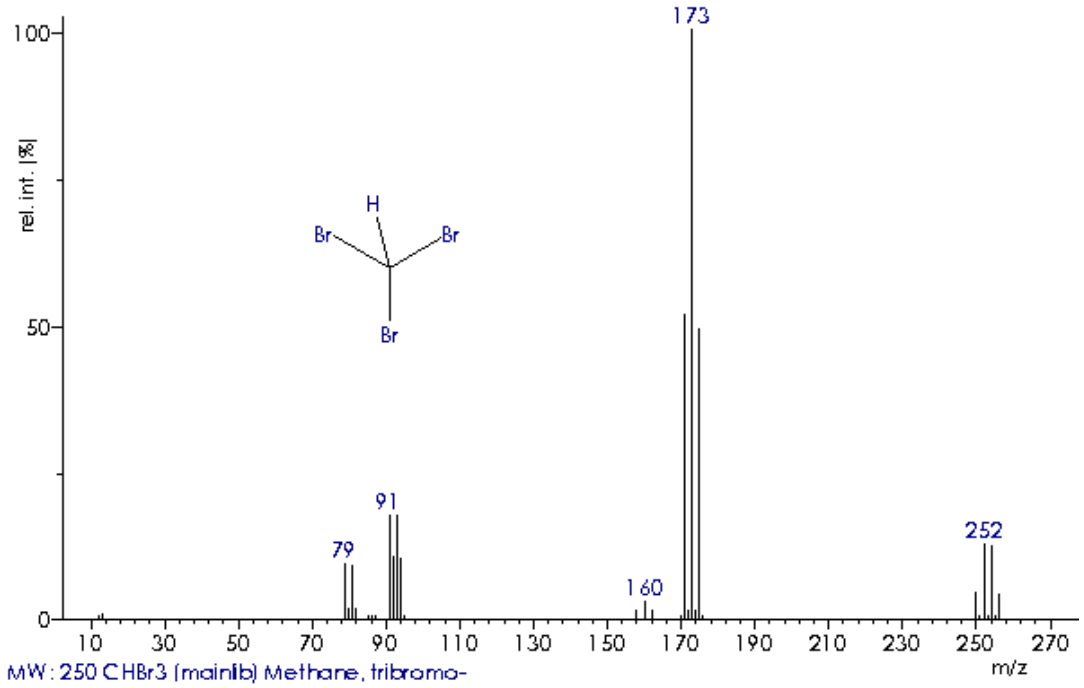
Answer 6.7

Identify the unknown from its 70 eV EI mass spectrum.



First, 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 at *m/z* 250 and exhibits a Br_3 isotopic pattern (250, 252, 254, 256). Even mass indicates 0, 2, 4, ... nitrogen atoms. ^{13}C peaks are very small, i.e., there are very few carbon atoms.

m/z 171, 173, 175	Br_2 pattern, $[M–79] \rightarrow [M–Br]^+$
m/z 158, 160, 162	Br_2 pattern $\rightarrow Br_2^{+\bullet}$
m/z 92, 94	Br pattern, $[M–158] \rightarrow [M–Br_2]^{+\bullet}$
m/z 91, 93	Br pattern, $[M–159] \rightarrow [M–Br–HBr]^+$
m/z 80, 82	Br pattern $\rightarrow HBr^{+\bullet}$
m/z 79, 81	Br pattern $\rightarrow Br^+$

As we have 3 bromines, the remaining mass of the unknown is 250 u – 3 × 79 u = 13 u which should correspond to CH.
Thus, the molecular formula most probably is $CHBr_3$; r+d = 1 – 0.5 × (1 + 3) +1 = 0

There is only one reasonable isomer of bromoform.

Fragmentation scheme (analogous to CH_4 and CH_3I):