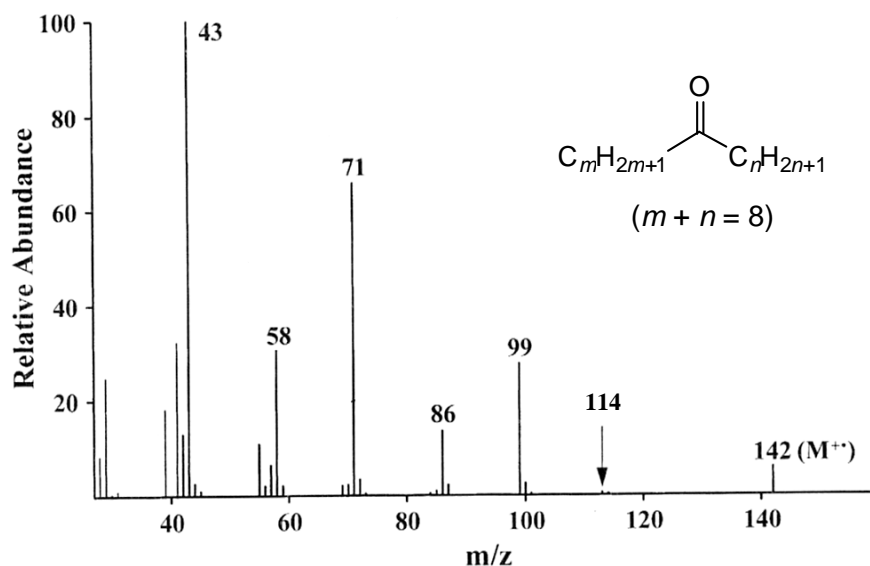


**In-Class Exercise:
Ketone Radical Cation Fragmentation**

The EI-MS shown below is of a ketone with molecular formula $C_9H_{18}O$ (obtained from its exact mass, measured by high-resolution mass spectrometry). The goal of this exercise will be to determine the structure of this ketone.



- All of the labeled peaks in the spectrum can be derived from one radical cation parent. What is the most likely parent ion structure? (Which single electron is most easily ejected from the ketone?)
- Some of the daughter peaks come from α -cleavage of this parent. Which ones? Draw a mechanism (push single-headed arrows) for each daughter.
- Some other daughter peaks come from McLafferty rearrangement of the parent. Which ones? Again, draw a mechanism for each.
- The peaks at $m/z = 43$ and 58 each come from sequential fragmentation of daughter ions that you drew in parts *b* and *c*. How?
- What is the structure of the ketone?