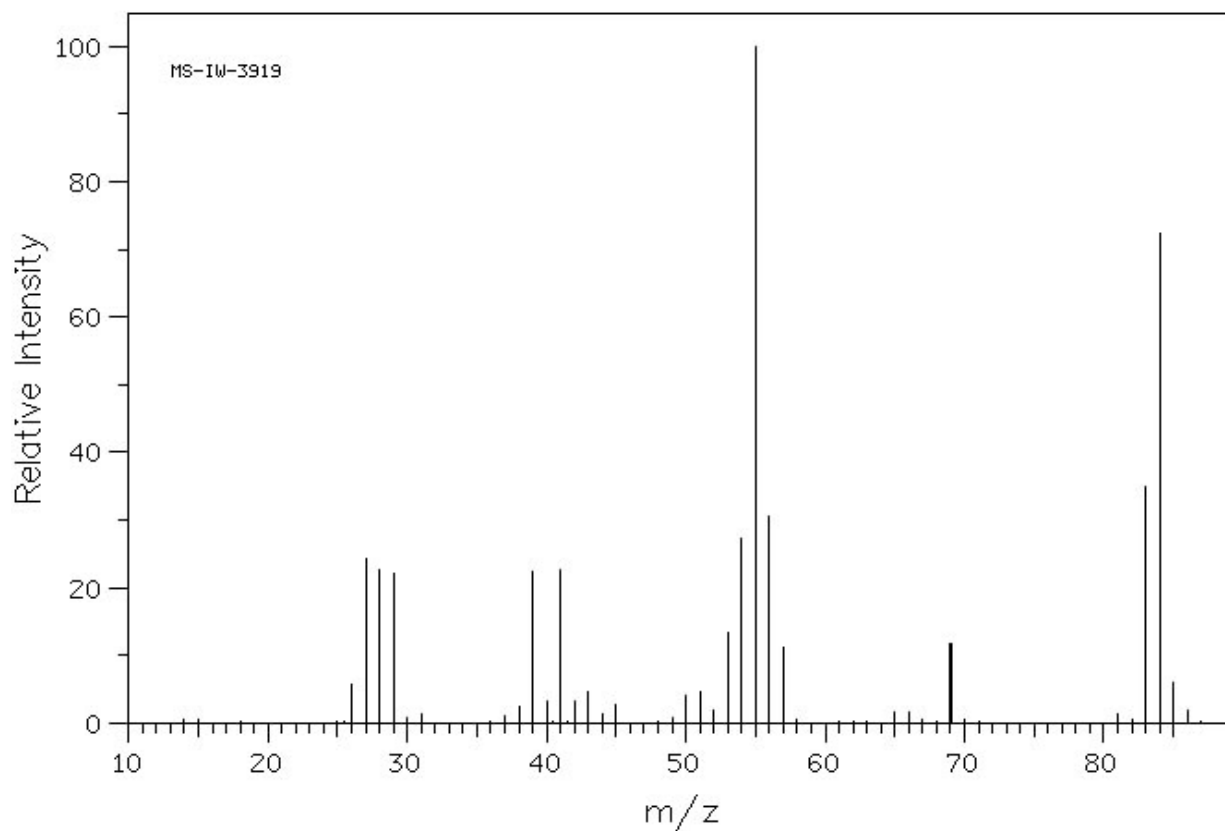


Exercise 1: Mass spectroscopy and infrared spectroscopy

1. The mass spectrum for a compound with formula C_xH_yO is given below



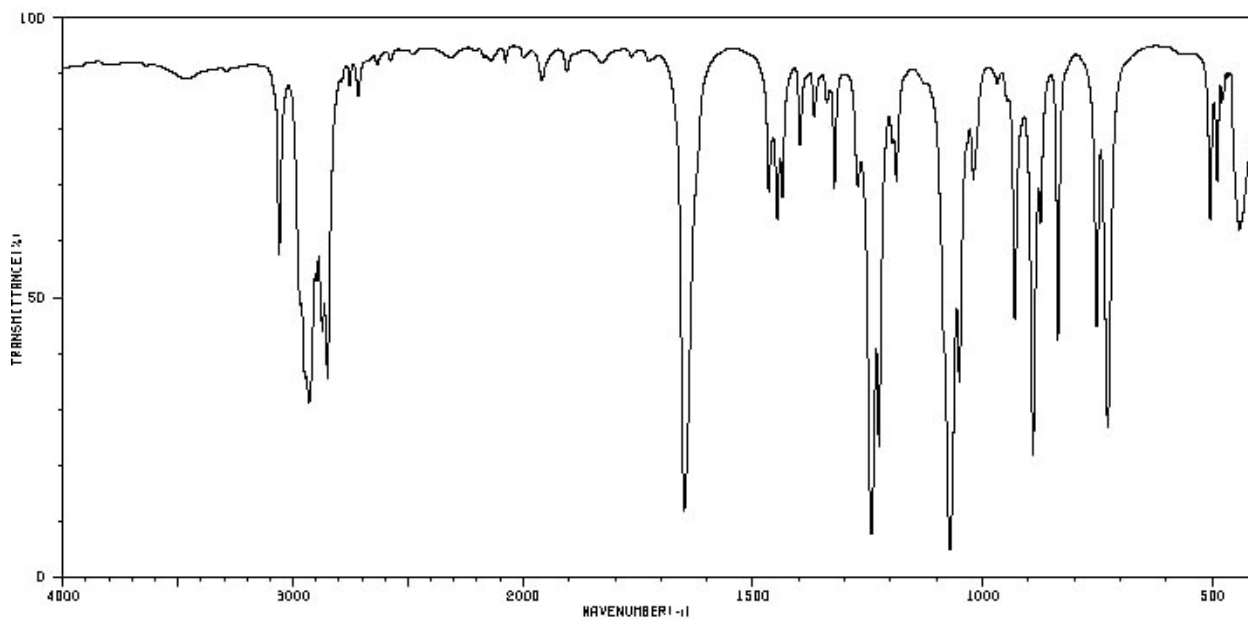
m/z	intensity	m/z	intensity
26	5.8	51	4.5
27	24.3	52	2
28	22.7	53	13.3
29	22.2	54	27.4
31	1.3	55	100
37	1.1	56	30.5
38	2.4	57	11.1
39	22.5	65	1.5
40	3.2	66	1.5
41	22.7	69	11.6
42	3.3	81	1.3
43	4.7	83	34.8
44	1.3	84	72.5
45	2.7	85	6.1
50	4	86	1.9

a. What is the molecular mass of this compound?

b. Calculate the number of carbons in this compound.

c. Using Appendix VI, give a plausible identity for the peaks at $m/z = 27$ and at the base peak.

d. The infrared spectrum for the same compound is given below.



3464	86	2763	84	1367	79	1188	68	874	60
3061	55	2716	84	1339	81	1071	4	836	41
2947	34	1649	11	1323	86	1051	39	752	43
2930	30	1466	66	1272	66	1020	68	728	26
2898	50	1447	62	1243	7	969	84	506	62
2872	42	1438	66	1226	22	930	44	490	66
2850	34	1398	74	1197	74	891	21	442	60

Give peak assignments (functional and other groups) for the following peaks:

Wavenumber (cm ⁻¹)	Functional or other group	Bend or stretch?
2930		
1649		
1243		
1070		

e. How do you know that there is *not* a carbonyl-containing group in this molecule?

f. Draw a reasonable structure for this compound.

2. The IR spectra below are for 2,2,4-trimethylpentane, 1-pentene and n-pentane. Assign each spectrum to the correct compound, and justify your choice, giving specific peak assignments.

