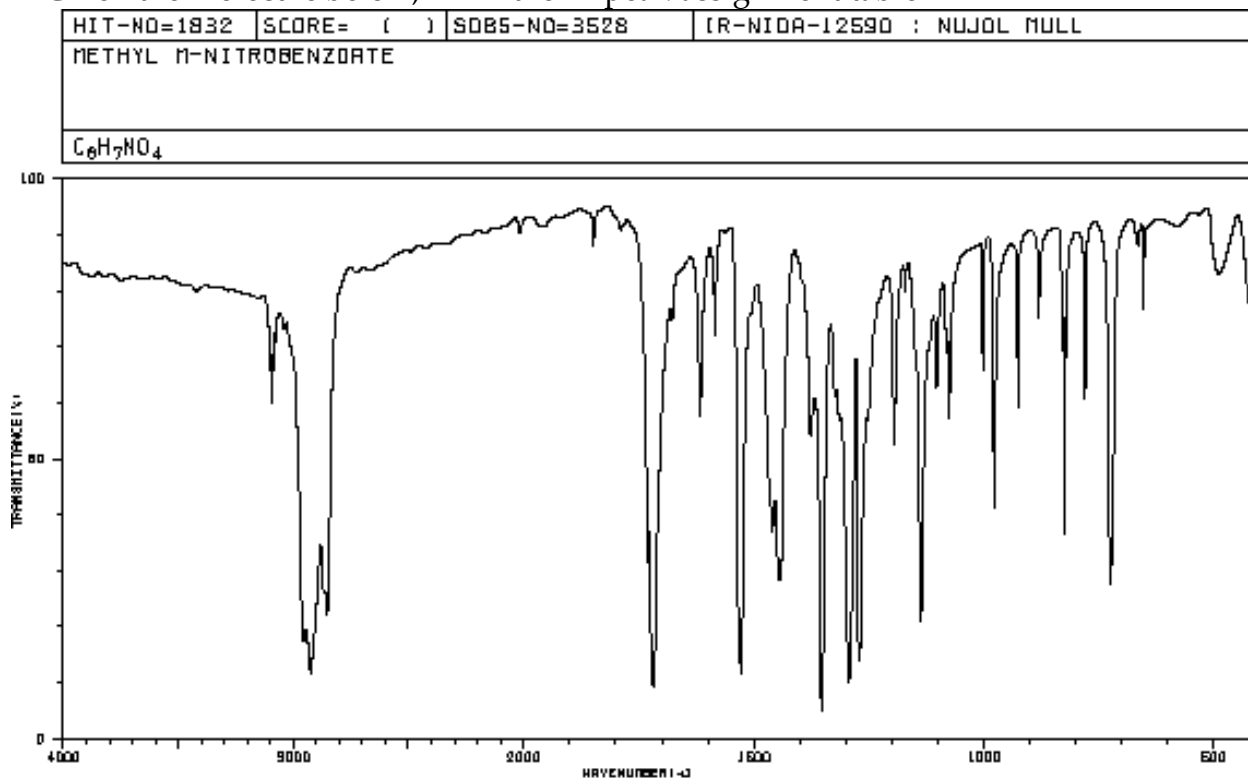


Exercise 2: Characterization of compounds using spectroscopic techniques

1. Given the molecule below, fill in the IR peak assignment table:



3092	66	1751	90	1480	36	1195	50	926	57
3082	86	1719	8	1444	26	1137	20	881	72
3042	70	1678	72	1377	62	1103	50	830	56
2966	17	1616	66	1362	4	1082	66	826	36
2924	11	1606	70	1293	9	1076	66	781	68
2868	26	1632	13	1272	13	1002	64	726	26
2864	21	1627	11	1259	66	978	39	663	74

Peak (cm ⁻¹)	Bond assignment	Mode (stretch or bend?)
2966-2924		
1719		
1527, 1362		
1137		
826-600		

2. a. Assign "cis" or "trans" to the following isomers of 1,3-dibromo-1,3-dimethylcyclobutane, based on their $^1\text{H-NMR}$ spectrum descriptions below:

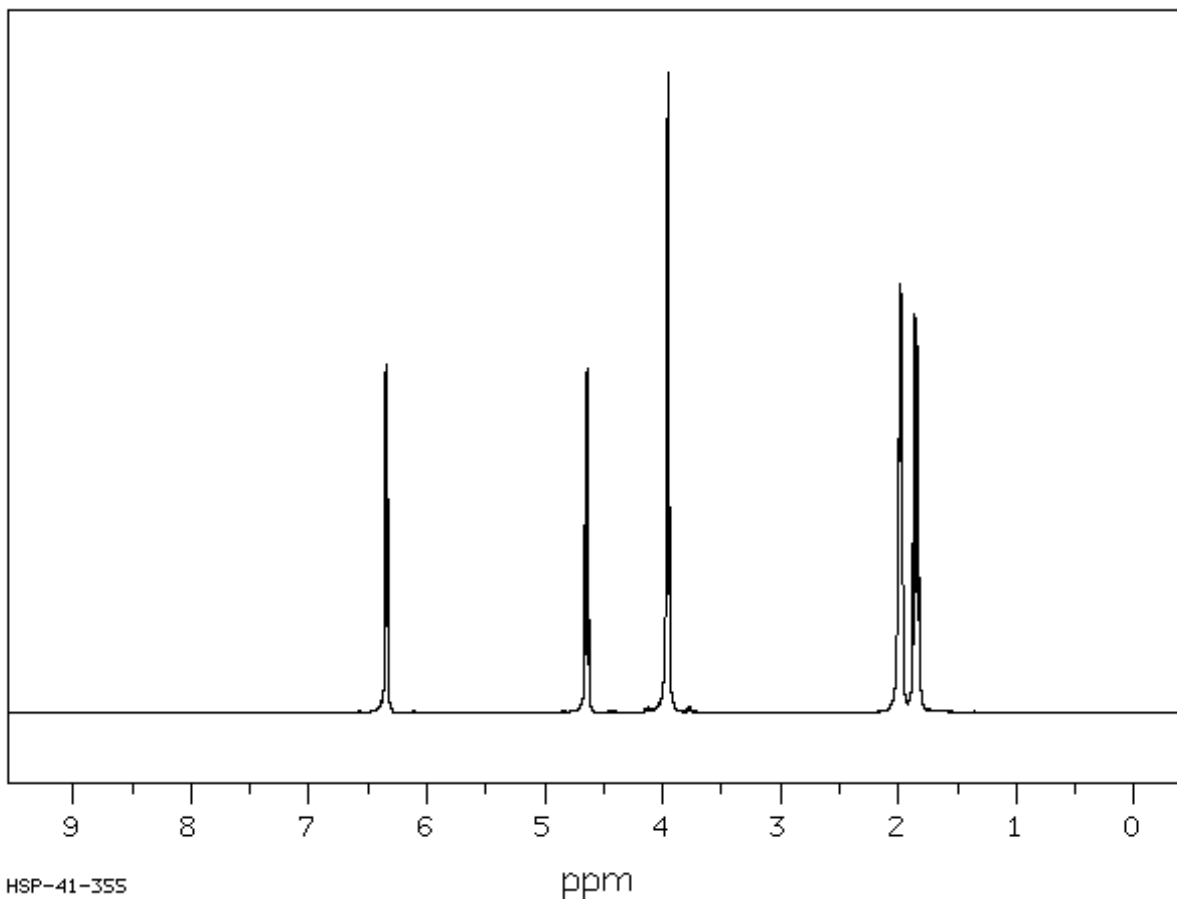
Isomer X: singlet, δ 2.13, integration area = 27
 singlet, δ 3.21, integration area = 18

Isomer Y: singlet, δ 1.88, integration area = 27.6
 doublet, δ 2.84, integration area = 9.2
 doublet, δ 3.54, integration area = 9.2

The doublets both have equal spacing.

b. Draw the structure of each isomer and label each group of equivalent peaks with the appropriate NMR signal.

3. Recalling exercise 1, problem 1, this is the ^1H -NMR of that compound, and their chemical shifts.



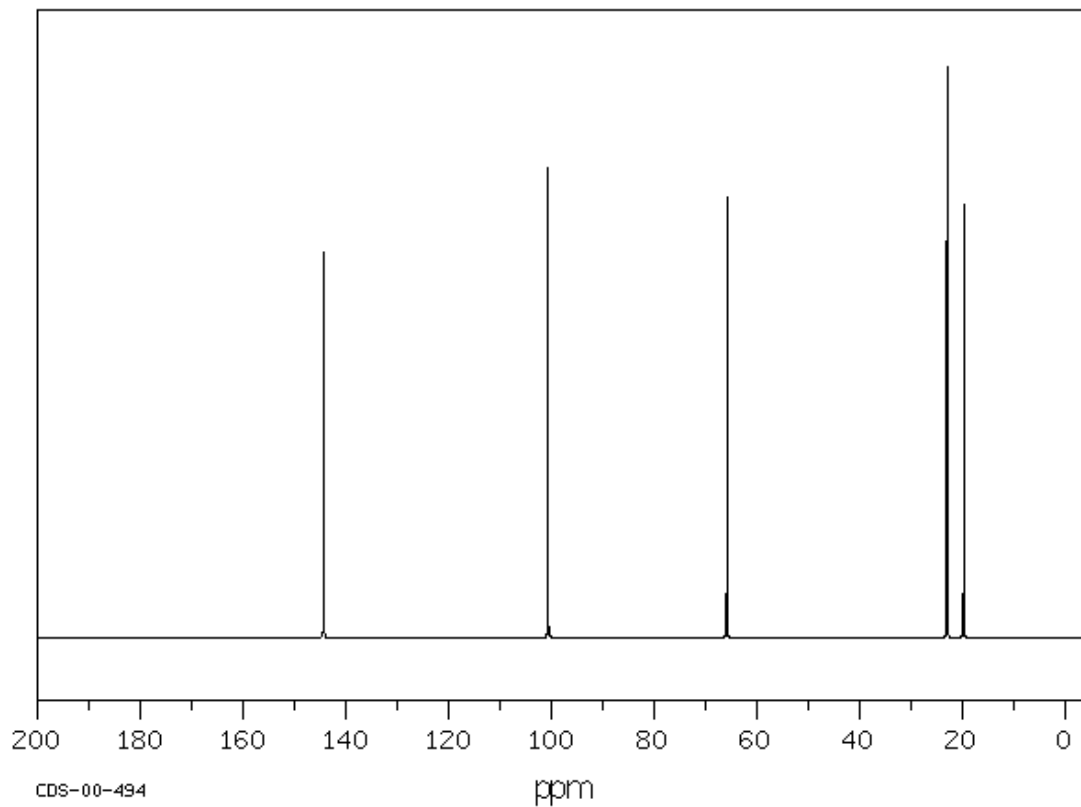
Assign.	Shift (ppm)	Integration	Splitting
A	6.342	1	doublet
B	4.644	1	complex multiplet
C	3.957	2	triplet
D	1.984	2	complex multiplet
E	1.846	2	complex multiplet

a. How many sets of equivalent protons are there?

b. Explain the splitting of peaks A and C – in other words, how many protons are on the carbon adjacent to those peaks' carbons?

c. Given the information from exercise 1, propose a structure for the compound and assign the peaks to equivalent sets of hydrogens (use the letter designation given).

d. The spectrum below is the proton-decoupled ^{13}C -NMR. Draw the structure of the molecule and assign the peaks to the appropriate carbon. Give a short justification for each assignment.



ppm	Int.	Assign.
144.32	675	1
100.67	822	2
65.84	771	3
23.01	1000	4 *
19.74	758	5 *