

3. This question is about Double Bond Equivalents, DBE

- (a) (i) C_nH_{2n} 1/2
 (ii) C_nH_{2n-2} 1/2
 (iii) C_nH_{2n-2} 1/2
 (iv) C_nH_{2n-6} 1/2

(b)

| DBE = 3 | Ring | Double Bond | Triple Bond |
|------------|------|-------------|-------------|
| | 3 | 0 | 0 |
| | 2 | 1 | 0 |
| | 1 | 2 | 0 |
| | 1 | 0 | 1 |
| | 0 | 3 | 0 |
| | 0 | 1 | 1 |
| | | | |
| | | | |

If all correct (in any order) **2**
 Minus 1/2 mark for any missing or incorrect line down to 0

| DBE = 4 | Ring | Double Bond | Triple Bond |
|------------|------|-------------|-------------|
| | 4 | 0 | 0 |
| | 3 | 1 | 0 |
| | 2 | 2 | 0 |
| | 2 | 0 | 1 |
| | 1 | 3 | 0 |
| | 1 | 1 | 1 |
| | 0 | 4 | 0 |
| | 0 | 2 | 1 |
| | 0 | 0 | 2 |
| | | | |
| | | | |



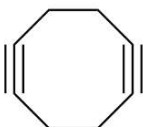
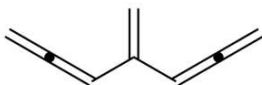
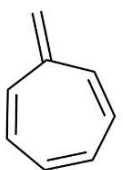
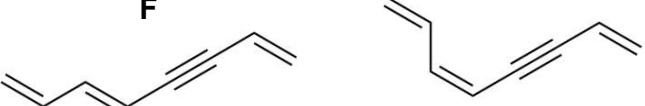
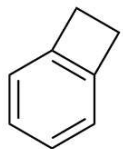
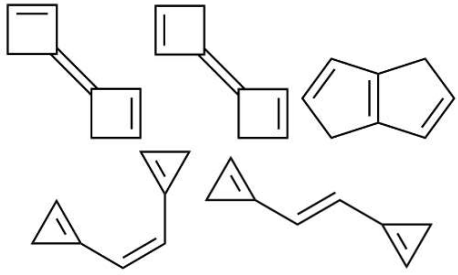
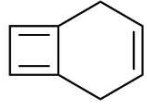
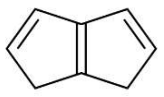
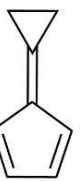

If all correct (in any order) **3**
 Minus 1/2 mark for any missing or incorrect line down to 0

- (c) (i) 4 1/2
 (ii) 9 1/2
 (iii) 61 1/2
 (iv) 4 1/2
 (v) 4 1/2
 (vi) 3 1/2

(d)

| Spectrum | Number of atoms in each region (must add to 8) | | | | | Structural information deduced | | | |
|----------|---|-------------------------|-------------|----------------|-----------------|--------------------------------|------------------------|-----------------|-----|
| | Triple Bond (Alkyne) | Double Bond (Alkene) | Single Bond | Allene Central | Allene Flanking | Number of Triple Bonds | Number of Double Bonds | Number of Rings | |
| A | 0 | 8 | 0 | 0 | 0 | 0 | 4 | 1 | 1/2 |
| B | 0 | 0 | 8 | 0 | 0 | 0 | 0 | 5 | 1/2 |
| C | 4 | 0 | 4 | 0 | 0 | 2 | 0 | 1 | 1/2 |
| D | 0 | 2 | 0 | 2 | 4 | 0 | 5 | 0 | 1 |
| E | 0 | 8 | 0 | 0 | 0 | 0 | 4 | 1 | 1/2 |
| F | 2 | 6 | 0 | 0 | 0 | 1 | 3 | 0 | 1/2 |
| G | 0 | 6 | 2 | 0 | 0 | 0 | 3 | 2 | 1/2 |
| H | 0 | 6 | 2 | 0 | 0 | 0 | 3 | 2 | 1/2 |
| I | 0 | 2 | 6 | 0 | 0 | 0 | 1 | 4 | 1/2 |

Each line must be fully correct to score the mark

| | | |
|---|--|---|
| <p style="text-align: center;">A</p>  | <p style="text-align: center;">B</p>  | 2 |
| <p style="text-align: center;">C</p>  | <p style="text-align: center;">D</p>  | 4 |
| <p style="text-align: center;">E</p>  | <p style="text-align: center;">F</p>  <p style="text-align: center;"><i>This is the correct structure</i> <i>This structure also fits the NMR data</i></p> | 4 |
| <p style="text-align: center;">G</p>  <p style="text-align: center;"><i>This is the correct structure</i></p> |  <p style="text-align: center;"><i>These structures also fit the NMR data</i></p>  <p style="text-align: center;"><i>This structure is unstable as is antiaromatic but also fits the NMR data so give full credit</i></p> | 2 |
| <p style="text-align: center;">H</p>  <p style="text-align: center;"><i>This is the correct structure</i></p>  <p style="text-align: center;"><i>This structure also fits the NMR data</i></p> | <p style="text-align: center;">I</p>  | 4 |

Structures A and B are worth 1 mark each, Structures C-I are worth 2 marks each. Marks are awarded for each fully correct structure in the correct place. Correct structures in an incorrect place score zero. No partial marks are awarded for a structure. No error carried forward is allowed if structure is wrong but consistent with the student's answer in the previous table. Where more there is more than one possibility only one structure needs to be drawn. There may be other possibilities which can be given full credit but only if they are **fully** consistent with all NMR data listed. Please contact the Committee if you find any alternatives.