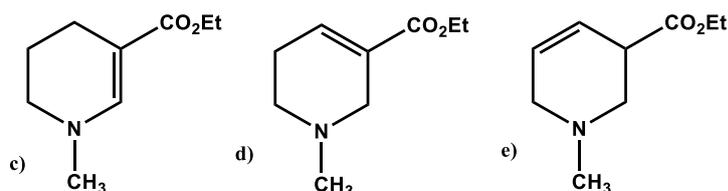
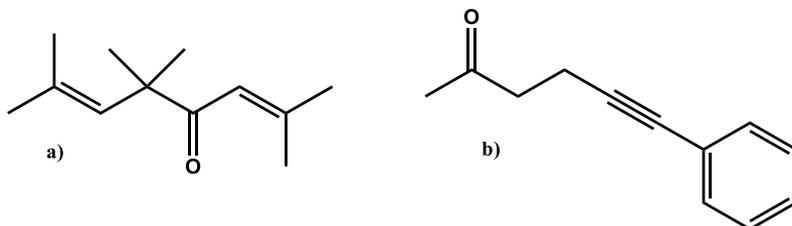


QFL0341 - Estrutura e Propriedades de Compostos Orgânicos Noturno (2019)  
5ª Lista de exercícios

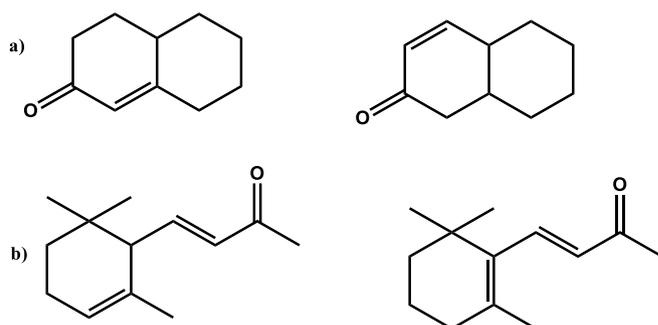
1) Qual alceno mais estável em cada par? Justifique.

- a) 2-metil-2-penteno ou 2,3-dimetil-2-buteno
- b) cis-3-hexeno ou trans-3-hexeno
- c) trans-2-hexeno ou 2-metil-2-penteno.

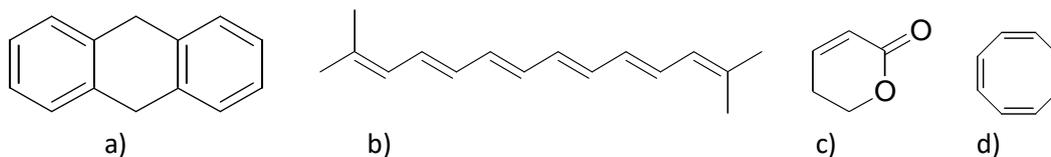
2) Represente estruturas de ressonância para os compostos abaixo.



3) Preveja e explique como a espectroscopia no UV-VIS pode ser utilizada para distinguir os seguintes pares de compostos. Reforce suas respostas com cálculos. Utilize as tabelas fornecidas ao final da Lista.

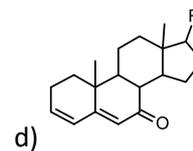
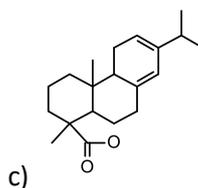
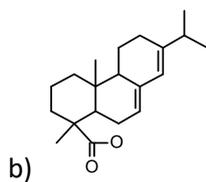


4) Quais dos compostos abaixo deve apresentar absorção na região visível do espectro eletromagnético?



5) Calcule os máximos de absorção para os compostos abaixo. Utilize as tabelas fornecidas a seguir.

a) 2,4-dimetil-1,3-pentadieno

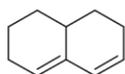


Regras de Woodward-Fieser para dienos

acyclic butadiene = 217 nm



Heteroannular (transoid):



base  $\lambda_{max} = 214$   
 $\epsilon = 5,000 - 15,000$

Homoannular (cisoid):

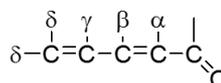
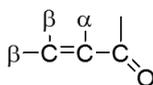


base  $\lambda_{max} = 253$   
 $\epsilon = 12,000-28,000$

The incremental contribution of substituents:

| Group                | Increment |
|----------------------|-----------|
| Extended conjugation | +30       |
| Each exo-cyclic C=C  | +5        |
| Alkyl                | +5        |
| -OCOCH <sub>3</sub>  | +0        |
| -OR                  | +6        |
| -SR                  | +30       |
| -Cl, -Br             | +5        |
| -NR <sub>2</sub>     | +60       |

Regras de Woodward-Fieser para enonas



| Group                             |                                    | Increment      |
|-----------------------------------|------------------------------------|----------------|
| 6-membered ring or acyclic enone  |                                    | Base 215 nm    |
| 5-membered ring parent enone      |                                    | Base 202 nm    |
| Acyclic dienone                   |                                    | Base 245 nm    |
| Double bond extending conjugation |                                    | 30             |
| Alkyl group or ring residue       | $\alpha, \beta, \gamma$ and higher | 10, 12, 18     |
| -OH                               | $\alpha, \beta, \gamma$ and higher | 35, 30, 18     |
| -OR                               | $\alpha, \beta, \gamma, \delta$    | 35, 30, 17, 31 |
| -O(C=O)R                          | $\alpha, \beta, \delta$            | 6              |
| -Cl                               | $\alpha, \beta$                    | 15, 12         |
| -Br                               | $\alpha, \beta$                    | 25, 30         |
| -NR <sub>2</sub>                  | $\beta$                            | 95             |
| Exocyclic double bond             |                                    | 5              |
| Homocyclic diene component        |                                    | 39             |

Referência:

Pavia, D., Lampman, G. M., Kriz, G. S. and Vyvyan, J. R. (2016) Introdução à Espectroscopia. Cengage Learning. Cap. 10. Espectroscopia no ultravioleta, páginas 559 – 594.