

Question #63710, Chemistry / Other

Calculate absorption spectra λ_{max} of diene, when the parent compound $H_2C=CH-CH=CH_2$ contains 3 methyl groups absorbs at 214 nm.

Solution:

CONJUGATED DIENE CORRELATIONS:

- i) Base value for homoannular diene = 253 nm
- ii) Base value for heteroannular diene = 214 nm
- iii) Alkyl substituent or Ring residue attached to the parent diene = 5 nm
- iv) Double bond extending conjugation = 30 nm
- v) Exocyclic double bonds = 5 nm
- vi) Polar groups: a) -OAc = 0 nm
b) -OAlkyl = 6 nm
c) -Cl, -Br = 5 nm

Thus:

Alkyl substituent = $3 \times 5 \text{ nm} = 15 \text{ nm}$

$$\lambda_{max} = 214 \text{ nm} + 15 \text{ nm} = \mathbf{229 \text{ nm}}$$

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