Ultraviolet-Visible (UV-Vis) Spectroscopy – Sample Problems Using Woodward-Fieser Rules

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Introduction

In this page we discuss a few examples of how we can utilize the **Woodward-Fieser** rules to determine the wavelength of maximum absorption for some molecules. We highly recommend that you read up the first two sections on the Woodward rules to calculate the λmax for conjugated dienes and the Woodward rules to calculate the λmax for unsaturated carbonyl compounds, before you read this page.

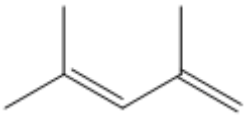
Note: Numerical values for Woodward-Fieser rules differ slightly from one textbook to another. We have tried to compile an extensive list of numerical values from online resources, textbooks and journal articles based on the popularity of the number. It is

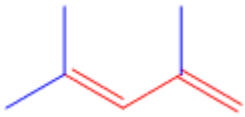
recommended that you learn on how to apply the values for the contributors and then follow the values given in a text book recommended by your teacher, or use our values. We believe that learning how to apply the rules is more essential than actually getting the exact answer. Other's opinions may vary.

In these sample problems you will be shown the structure, then the structure is highlighted to show you key features which would affect the λmax of the molecule. Then the table will show you the solutions on how to solve to get the wavelength of maximum absorption, with a final calculated λmax using the Woodward-Fieser rules. In some cases if we have an observed λmax for comparison, it may be given as well.

Note- If you have your own problems please write the IUPAC name in the comments section and I will attempt to solve it and add it to this list of examples.

Example/Sample Problem 1



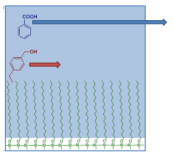


Name of Compound	2,4-dimethylpenta-1,3-diene
Woodward Component	Contribution
Core- Transoid/Heteroannular Diene	+ 215 nm
Substituents- 3 alkyl groups	3 x 5 = + 15 nm
Other Effects	0
Calculated λmax	230 nm
Observed λmax	234 nm

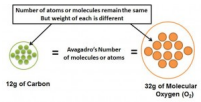
Example/Sample Problem 2

Ping Pong Mechanism of ...

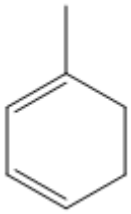
Digestion of Fats (Triacylglycerols)

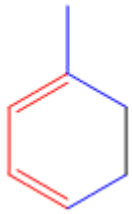


Principle of Reversed-Phase Chromatography HPLC/UPLC (with Animation)



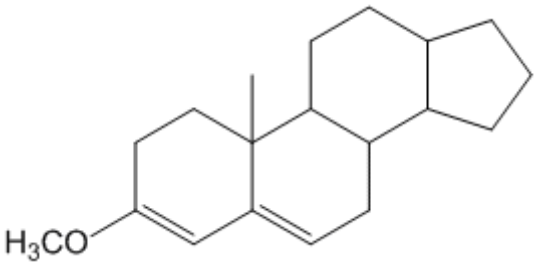
A Primer on Measuring Concentrations – Molarity, Moles and Other ...

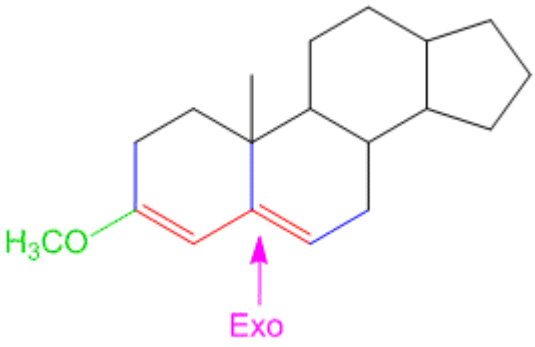




Name of Compound	1-methylcyclohexa-1,3-diene
Woodward Component	Contribution
Core- Cisoid/Homoannular Diene	+ 253 nm
Substituents- 3 alkyl groups	3 x 5 = + 15 nm
Other Effects	0
Calculated λmax	268 nm
Observed λmax	N/A

Example/Sample Problem 3

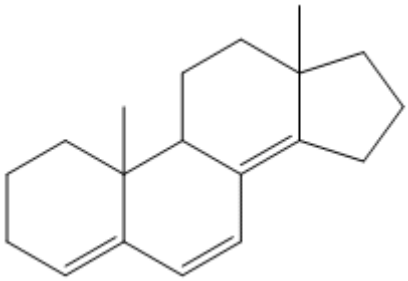


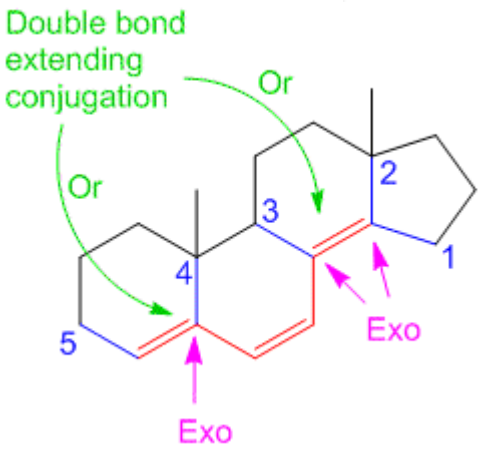


Name of Compound	3-methoxy-10-methyl-2,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene
Woodward Component	Contribution
Core- Transoid/Heteroannular Diene	+ 215 nm

Substituents- 3 alkyl groups	3 x 5 = + 15 nm
1 alkoxy group	+ 6 nm
Other Effects- Exocyclic Double Bond	+ 5 nm
Calculated λmax	**241 nm**
Observed λmax	N/A

Example/Sample Problem 4

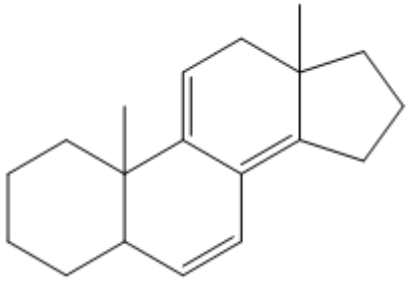




Name of Compound	10,13-dimethyl-2,3,9,10,11,12,13,15,16,17-decahydro-1H-cyclopenta[a]phenanthrene
Woodward Component	Contribution
Core- Transoid/Heteroannular	+ 215 nm
Substituents- 5 alkyl groups	5 x 5 = + 25 nm
1 Double bond extending conjugation	+ 30 nm
Other Effects- 3 Exocyclic Double Bond	+ 15 nm

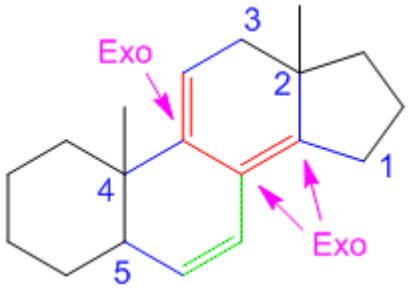
Calculated λmax	285 nm
Observed λmax	283 nm

Example/Sample Problem 5



Note- In this example the molecule contains both, a homoannular diene system and a heteroannular diene system. In such a molecule the core chromophore is considered to be the homoannular system and accordingly the calculations are performed.

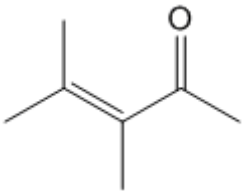
Homoannular system

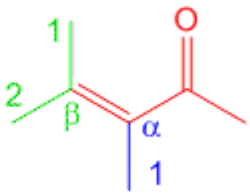


Component	Contribution
Core- Homoannular/Cisoid diene	+ 253 nm
Substituents– 5 alkyl substituents	5 x 5 = + 25 nm
Double bond extending conjugation	+ 30 nm

Other Effects- 3 Exocyclic double bonds	3 x 5 = + 15 nm
Calculated λ_{max}	323 nm
Observed λ_{max}	n/a

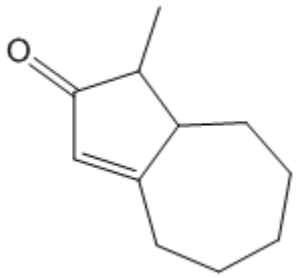
Example/Sample Problem 6

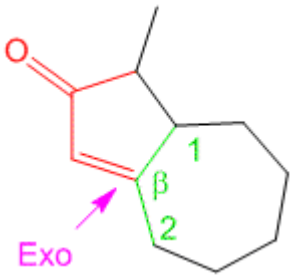




Name of Compound	3,4-dimethylpent-3-en-2-one
Component	Contribution
Core- α,β-unsaturated ketone	+ 215 nm
Substituents at α-position- 1 alkyl group	+ 10 nm
Substituents at β-position- 2 alkyl groups	2 x 12 = 24 nm
Other Effects	0
Calculated λ_{max}	249 nm
Observed λ_{max}	249 nm

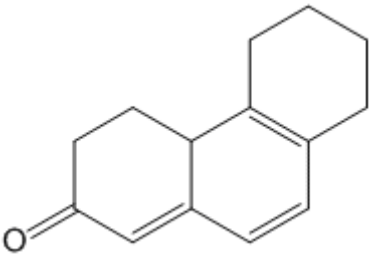
Example/Sample Problem 7

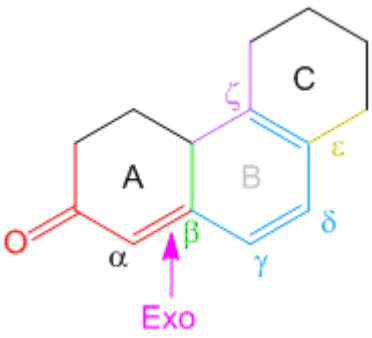




Name of Compound	1-methyl-4,5,6,7,8,8a-hexahydroazulen-2(1H)-one
Component	Contribution
Core- cyclopentenone	+ 202 nm
Substituents at α-position	0
Substituents at β-position- 2 alkyl groups	2 x 12= + 24 nm
Other Effects- 1 Exocyclic Double Bond	+ 5 nm
Calculated λ_{max}	231 nm
Observed λ_{max}	226 nm

Example/Sample Problem 8





Name of Compound	4,4a,5,6,7,8-

Name of Compound	4,4a,5,6,7,8-hexahydrophenanthren-2(3H)-one
Component	Contribution
Core- cyclohexenone	+ 215 nm
Substituents at α-position:	0
Substituents at β-position: 1 alkyl group	+ 12 nm
Substituents at γ-position:	0
Substituents at δ-position:	0
Substituents at ε-position: 1 alkyl group	+ 18 nm
Substituents at ζ-position: 2 alkyl group	2 x 18 = + 36 nm
Other Effects: 2 Double bonds extending conjugation	2 x 30 = + 60 nm
Homoannular Diene system in ring B	+ 35 nm
1 Exocyclic double bond	+ 5 nm
Calculated λ_{max}	**381 nm**
Observed λ_{max}	388 nm

Note- If you have your own problems please write the IUPAC name in the comments section and I will attempt to solve it and add it to this list of examples.

Example/Sample Problems For β-Carotene and all-trans-lycophene