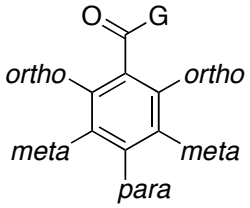
UV-VIS Calculation Tables

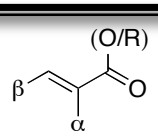
Base value for heteroannular diene	214
Base value for homoannular diene	253
Increments for	
Double bond extending conjugation	+30
Alkyl substituent or ring residue	+5
Exocyclic double bond	+5
Polar groupings: OAc	+0
OAlk	+6
SAlk	+30
Cl, Br	+5
$N(Alk)_2$	+60
Solvent correction[b]	+0
λ_{calc} = Total	

[a]See L. M. Fieser and M. Fieser, *Steroids*. New York: Reinhold, 1959, pp. 15–24; R. B. Woodward, *J. Am. Chem. Soc.*, **63**, 1123 (1941); **64**, 72, 76 (1942); A. I. Scott, *Interpretation of the Ultraviolet Spectra of Natural Products*. New York: Pergamon (Macmillan), 1964.

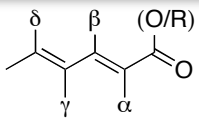
[b]Solvents have negligible effects upon the λ_{max} of these $\pi \rightarrow \pi^*$ transitions.



ArCOR/ArCHO/$ArCO_2H$/$ArCO_2R$		λ_{max}^{EtOH} (nm)
Parent chromophore: Ar = C_6H_5		
G = Alkyl or ring residue, (e.g., ArCOR)		246
G = H, (ArCHO)		250
G = OH, OAlk, ($ArCO_2H$ and $ArCO_2R$)		230
Increment for each substituent on Ar:		
—Alkyl or ring residue	o-, m-	+3
	p-	+10
—OH, —OCH_3, —OAlk	o-, m-	+7
	p-	+25
—O^- (oxyanion)	o-	+11
	m-	+20
	p-	+78[b]
—Cl	o-, m-	+0
	p-	+10
—Br	o-, m-	+2
	p-	+15
—NH_2	o-, m-	+13
	p-	+58
—$NHCOCH_3$	o-, m-	+20
	p-	+45
—$NHCH_3$	p-	+73
—$N(CH_3)_2$	o-, m-	+20
	p-	+85



enone



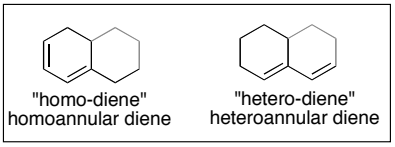
dienone

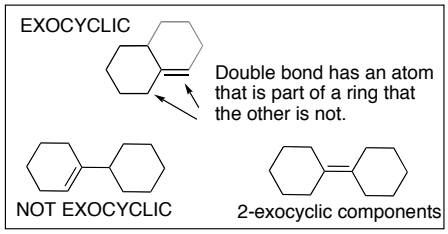
Base values	(nm)
Acyclic α,β-unsaturated ketones	215
Six-membered cyclic α,β-unsaturated ketones	215
Five-membered cyclic α,β-unsaturated ketones	202
α,β-Unsaturated aldehydes	210
α,β-Unsaturated carboxylic acids and esters	195
Increments for	
Double bond extending conjugation	+30
Alkyl group, ring residue α	+10
β	+12
γ and higher	+18
Polar groupings: —OH α	+35
β	+30
δ	+50
—OAc α,β,δ	+ 6
—OMe α	+35
β	+30
γ	+17
δ	+31
—SAlk β	+85
—Cl α	+15
β	+12
—Br α	+25
β	+30
$—NR_2$ β	+95
Exocyclic double bond	+5
Homodiene component[a]	+39
Solvent correction (see table below)	Variable
λ_{calc} = Total[b]	

[a]Two conjugated double bonds, both in the same ring.

[b]The calculated values usually fall within ±3 nm of the observed values. The molar absorptivities of *cisoid* enones are usually less than 10,000, whereas the molar absorptivities of *transoid* enones are greater than 10,000.

Terminology





J. Koh --adapted from Silverstein and Webster "Spectrocopic Identification of Organic Compounds, Wiley , 1998.