

A Spectral Comparison of 2-Quinolones with 2-Alkoxyquinolines

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Changes in structural features within a series of chemically related compounds can be correlated with changes in the electronic absorption spectra of these same compounds. This study involves the ultraviolet spectra-structure correlation for a series of 2-quinolones and 2-alkoxyquinolines.

Experimental

All spectra were determined at a constant temperature of 20°C. using a Bausch and Lomb Spectronic 505 recording spectrophotometer. The solvent was spectrally pure 95 per cent ethanol. The spectral range covered was from 205 to 350 millimicrons. The wave length reading of the instrument was calibrated using a mercury source; absorbance readings were checked at the various wave lengths using standard solutions of KNO_3 and K_2CrO_4 .

Samples of each solid compound were purified by repeated recrystallization to a constant melting point range of 1° C. Liquids were fractionated to a constant boiling temperature. The melting points and the boiling temperatures agreed with literature values. Stock solutions of each compound were prepared by weighing followed by dilution with spectrally pure 95 per cent ethanol to a known volume. Aliquots of these stock solutions were further diluted with the solvent to a spectrophotometrically feasible concentration range. The ultraviolet spectrum of each compound was determined at several different concentrations. This technique checked instrument reproducibility as well as the validity of the Beer-Lambert Law for the molecule.

Results and Discussion

Table 1. summarizes the spectral features for the series of molecules studied. Region A describes the spectral features below 215 millimicrons, region B features between 215 to 240 millimicrons, region C features between 240 and 260 millimicrons, region D features between 260 and 300 millimicrons, and region E spectral characteristics above 300 millimicrons.

In this series of compounds the only ultraviolet spectrums that are reported in the recent literature are for 2-quinolone, 4-methyl-2-quinolone, and 1-methyl-2-quinolone. The results that are quoted for these molecules in Table 1. agree closely to those in the literature (1, 2, 3). The absorption maximum in the region of 210 millimicrons is previously unreported. As yet no attempt has been made to identify the different

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TABLE 1
Spectral Characteristics of 2-Quinolones and 2-Alkoxy Quinolines in 95 Per Cent Ethanol

Compound	Wave Length in μ , and Log ϵ				
	A	B	C	D	E
2-quinolone	210(4.43)	228(4.63)	245(3.83) s	268(3.85)	316(3.74) s
				276(3.80) s	328(3.83)
					340(3.63) s
4-methyl-2-quinolone	210(4.42)	230(4.59)	243(4.06) s	267(3.82)	315(3.77) s
				276(3.78) s	325(3.86)
					337(3.72) s
3-methyl-4-ethyl-2-quinolone	215(4.50) s	221(4.56)	246(3.92) s	264(3.79) s	315(3.82) s
				270(3.88)	325(3.90)
				279(3.77)	338(3.75)
3-ethyl-4-propyl-2-quinolone	217(4.42) s	222(4.53)	247(3.93) s	264(3.78) s	315(3.82) s
				271(3.90)	325(3.92)
				281(3.82)	340(3.77)
3-propyl-4-butyl-2-quinolone	215(4.42) s	225(4.50)	247(3.90) s	265(3.78) s	316(3.82) s
				272(3.89)	326(3.92)
				281(3.80)	340(3.84)
3-butyl-4-pentyl-2-quinolone	216(4.52) s	223(4.57)	245(4.02) s	264(4.02) s	316(3.86) s
				272(3.95)	326(3.97)
				281(3.88)	339(3.82)
4,8-dimethyl-2-quinolone	212(4.39) s	232(4.55)	247(4.23)	273(3.88)	318(3.68) s
				281(3.84) s	329(3.76)
					340(3.67) s
3-bromo-4-methyl-2-quinolone	212(4.39) s	232(4.55)	247(4.23)	270(3.81) s	321(3.80) s
				277(3.90)	332(3.90)
				287(3.83)	346(3.76)
1-methyl-2-quinolone	212(4.39) s	229(4.59)	245(3.86) s	270(3.84)	320(3.71) s
				278(3.82)	330(3.87)
					340(3.67) s

TABLE 1 (continued)
Spectral Characteristics of 2-Quinolones and 2-Alkoxy Quinolines in 95 Per Cent Ethanol

Compound	Wave Length in μ . and Log ϵ				
	A	B	C	D	E
1,4-dimethyl-2-quinolone		230(4.60)	243(4.06)	269(3.89) 277(3.78)	318(3.74)s 327(3.80) 339(3.65)s
1,3-dimethyl-4-ethyl-2-quinolone		228(4.57)	246(3.96)s	266(3.76)s 273(3.88) 282(3.74)	317(3.80)s 326(3.84) 339(3.68)s
1-methyl-4-formyl-2-quinolone	213(4.46)s	229(4.55)	247(4.01)s	272(3.82) 279(3.78)	320(3.74)s 331(3.80) 343(3.65)s
2-methoxyquinoline	209(4.56)	225(4.56) 231(4.56)	256(3.81)	264(3.77)s 277(3.55)s 296(3.46)	304(3.51)s 308(3.55) 317(3.55)
2-methoxy-4-methyl-quinoline	215(4.48)s	222(4.57)s 226(4.59)	248(3.59) 258(3.63)	267(3.63) 276(3.49)s 296(3.30)s	321(3.51) 308(3.55) 322(3.59)
2-ethoxy-4,8-dimethyl-quinoline	209(4.62)	232(4.68) 238(4.47)		272(3.75) 284(3.57)s 300(3.32)s	311(3.51) 325(3.55)
2-methoxy-4,6,8-trimethyl-quinoline	212(4.63)	232(4.67) 238(4.67)		264(3.74) 273(3.72)	306(3.33)s 318(3.55) 332(3.58)

absorption bands with particular electronic transitions. However, it appears that the following spectra-structure correlations can be made:

1. 3,4-Disubstitution is characterized by its absorption features in regions D and E. In region D normal alkyl substitution in the 2-quinolone molecule shows a maximum-shoulder characteristic; 3,4-disubstitution shows a shoulder maximum-maximum feature. In region E the normal alkyl-substituted 2-quinolone spectrally shows a shoulder-maximum-shoulder feature; 3,4-disubstitution shows a shoulder-maximum-maximum feature. The replacement of an alkyl group by bromine in the 3-position produces the expected bathochromic shift but does not destroy the 3,4-disubstitution characteristic.

2. Alkyl substitution on the N atom spectrally shows a maximum-maximum feature in region D instead of a maximum-shoulder feature seen in the case of normal alkyl substitution.

3. 2-Alkoxyquinolines are characterized by a double maximum in region B instead of the single maximum characteristic of the 2-quinolones. In region E the ethers have a maximum-maximum feature at the longest two wave lengths instead of the shoulder-maximum-shoulder feature of the 2-quinolones.

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