chelating sulfato groups—around the linear OUO group.

Registry No. $UO_2(phen)SO_4$, 42565-88-8; $UO_2(2,2'\text{-bpy})SO_4$, 40415-75-6; $UO_2(2,2'\text{-bpyO}_2)SO_4$, 50989-29-2; $UO_2(4,4'\text{-bpy})SO_4$, 51024-41-0; $UO_2(2,2'\text{-bpyA})_2SO_4$, 63162-30-1; $UO_2(4,4'\text{-bpyO}_2)SO_4$, 96789-83-2; $UO_2(MP)SO_4$, 76772-31-1; $UO_2(Q)_2SO_4$, 73689-28-8; $UO_2(DMQ)_2SO_4$, 73700-17-1; $UO_2(HMTA)_2SO_4$, 71769-14-7; $UO_2(DPP)SO_4$, 60647-93-0; $UO_2(MBT)SO_4$, 68229-42-5; $UO_2(NA)_2SO_4$, 67799-02-4.

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Spectroscopic Study of Some New *N*-Aryl Pyrroles

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A series of new 2,5-dimethyl-N-substituted pyrroles (I) were obtained by condensation of 2,5-hexanedione with different amines. The UV data show that about 11.7% of the total electronic density of the nitrogen of pyrrole ring is conjugated with the aryl group. A correlation between the UV and NMR results has been established, and the mass spectra of these derivatives have also been measured and discussed.

Introduction

It is well-known that alkylated and N-alkylated pyrroles were obtained from condensation between 2,5-hexanedione and amines (*1*). The UV (*1*, *2*), IR, and NMR spectra (*1*, *3*) and mass fragmentation (*1*, *4*, *5*) of pyrrole and some of its derivatives have been investigated previously. Our N-substituted pyrroles series allows us to establish a correlation study between the UV and NMR, a study not previously attempted on pyrroles. The mass spectra of these derivatives have also been measured.

Results and Discussion

The position of CH_3 groups in the NMR spectra (Table I) of Ib (δ = 2.008) and Id (δ = 1.930) are shifted to a higher field compared with that of Ia (δ = 2.090) owing to the conjugation of the nitrogen electron pair with the π-conjugated system of the phenyl ring. *N*-Aryl substitution causes a red shift of the long UV band (Table I) by about the same amount, 28 ± 3 nm, which probably means that only 28/240 = 0.117 or 11.7% of the total electronic density of the nitrogen electrons is conjugated with the aryl ring.

The long UV bands of all compounds are red-shifted in concentrated sulfuric acid by the same amount (Table I); in this medium withdrawal of the nitrogen electron lone pair should occur and the spectrum may represent a charged aminodiene (*6*).

The mass spectra of compounds Ia–e are shown in Table II in the form of relative intensities vs. *m/z*.

Table I. ^1H NMR Data and UV Absorption Bands of 2,5-Dimethyl-N-substituted Pyrroles in Ethanol and Concentrated Sulfuric Acid

	NMR data			UV bands [λ_{max}, nm (log ϵ, m^2 mol^{-1})]	
molecule	δ, ppm	intens	multipl	EtOH	concd H_2SO_4
pyrrole[a]				240 (2.48)	
				210 (3.70)	
Ia	0.84	3	triplet	226 (2.10)[b]	242 (2.46)
	1.61	2	sextet	208 (2.30)	202 (2.21)
	2.09	6	singlet		
	3.55	2	triplet		
	5.62	2	singlet		
Ib	2.008	6	singlet	264 (2.31)	284 (2.73)
	5.88	2	singlet	230 (3.05)[b]	240 (2.86)
	7.20–7.33	5	complex	213 (2.23)	205 (3.12)
Ic	2.010	6	singlet	271 (2.04)[b]	294 (2.51)
	3.85	3	singlet	234 (3.03)	235 (2.64)[b]
	5.87	2	singlet	209 (3.02)	222 (2.70)
	6.91–7.23	4	complex		
Id	1.93	6	singlet	266 (2.40)	288 (2.72)
	5.79	2	singlet	243 (3.03)	242 (2.83)
	6.88–6.98	2	doublet	218 (3.28)	219 (3.07)
	7.23–7.32	2	doublet		
Ie				270 (3.23)	291 (3.35)
				204 (3.16)	208 (2.90)

[a] From ref 2. [b] Shoulder.

Experimental Section

Compound Ia (Figure 1) was prepared by refluxing, for 90 min equimolar amounts of *n*-propylamine and 2,5-hexanedione;

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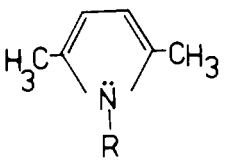
Table II. *m/z* of Major Peaks with Their Relative Intensities Observed in the Mass Spectra of Compounds Ia–e[a]

Ia		Ib		Ic		Id		Ie			
m/z	rel intens	*m/z*	rel intens	*m/z*	rel intens	*m/z*	rel intens	*m/z*	rel intens	*m/z*	rel intens
39	14	51	15	39	5	39	7	39	18	121	9
41	24	77	23	63	5	50	5	41	14	128	11
42	21	115	5	64	5	51	10	42	11	129	5
43	7	128	9	65	5	52	6	50	6	130	10
51	8	129	6	77	8	53	7	51	26	131	7
52	8	130	5	92	5	72	5	52	7	132	5
										141	6
53	14	154	10	100	8	75	15	53	16	143	6
54	13	156	11	117	6	77	6	55	5	144	18
55	6	168	5	145	22	83	14	56	5	146	58
65	7	170	100	154	6	84	7	63	7	147	10
66	6	171[c]	79	156	5	111	14	65	9	154	24
67	14	172	10	159	7	113	5	66	5	155	5
77	7			160	5	127	5	67	5	156	18
79	7			186	20	128	7	76	5	157	9
80	9			200	65	129	26	77	48	158	21
92	7			201[c]	100	154	25	78	10	159	5
93	9			202	16	155	10	79	9	167	33
94	71					167	8	80	5	168	68
95	24					168	13	81	13	169	16
106	6					169	17	83.5[b]	14	170	26
107	8					170	5	89	8	171	5
108	100					190	10	90	8	172	21
109	37					204	100	90.5[b]	9	180	9
120	6					205[c]	95	91	11	181	10
122	23					206	45	91.5[b]	8	182	48
136	35					207	34	92	8	183	22
137[c]	82									184	11
138	11							93	22	186	43
								94	11	187	5
								96	24	200	37
								99.5[b]	9	201[c]	100
								100	8	202	38
								103	5		
								104	5		
								105	29		
								115	11		
								116	5		
								117	9		
								118	10		
								119	8		

[a] Peaks less than 5% are not included. [b] Doubly charged ion. [c] Parent peak.



Ia: R = n-C_3H_7
b: R = C_6H_5
c: R = C_6H_4(p-OCH_3)
d: R = C_6H_4(p-Cl)
e: R = C_6H_4(o-CH_2OH)

Figure 1. Structure of 2,5-dimethyl-N-substituted pyrroles.

the mixture was then fractionally distilled twice under reduced pressure and the fraction which boiled at 40 °C/0.3 torr was collected.

The other compounds, Ib–e, were prepared by refluxing equimolar amounts of the corresponding amine and the dione for 6 h. On freezing, a colorless to light brown crystalline product precipitated in every case; the precipitate was filtered and purified by sublimation under reduced pressure. Ib had mp 48–49 °C; Ic, 60–61 °C; Id, 46–48 °C; Ie, 105–107 °C. All the compounds gave satisfactory elemental analyses. The measurements of the spectra are discussed elsewhere (*7*, *8*).

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Registry No. Ia, 20282-39-7; Ib, 83-24-9; Ic, 5044-27-9; Id, 5044-23-5; Ie, 97690-10-3.

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