

Structure parameter correlation of some quinoxaline derivatives through IR and ^{13}C NMR spectra

G. Thirunarayanan^{1,*}, I. Muthuvel¹, V. Sathiyendiran²

¹Department of Chemistry, Annamalai University, Annamalainagar - 608 002, India

²Department of Chemistry, Sourashtra College, Madurai - 625 004, India

*E-mail address: drgtnarayanan@gmail.com

ABSTRACT

A series of 6-substituted quinoxaline derivatives have been synthesized and examined their purities by literature method. The infrared and ^{13}C NMR spectral data of these quinoxalines were correlated with Hammett substituent constants, F and R parameters using single and multi-regression analysis. From the results of statistical analysis, the effect of substituents on the spectral frequencies has been studied.

Keywords: Quinoxalines; IR spectra; NMR spectra; Hammett Correlation; Substituent effects

1. INTRODUCTION

Quinoxaline derivatives are medicinally important bi nitrogen heterocycles due to presence of this ring in numerous antibiotics [1,2]. The important biological activities of quinoxalines are antibacterial [2,3], antiviral [4], anti-inflammatory [4], askinase inhibitors [4], anticancer [4], antimycobacterial [5,6], antifungal [7], anthelmintic [4,7], antidepressants [8] and antitumour [9,10]. Many kinds of synthetic methods including solvent-free and catalysts were reported in the literature for synthesis of quinoxalines by the condensation of 1,2-diamines and 1,2-dicarbonyl compounds [1,2,11].

Spectroscopic data have been employed for studying the molecular equilibration of carbonyl compounds, pyrazolines and imines [12-14]. The E- and Z-notation of alkenes including α,β -unsaturated carbonyl compounds and the stereochemistry of protons in the pyrazoline derivatives are confirmed by IR and ^1H NMR spectroscopy [12-14]. The qsar and qspr study was established with various compounds such as chalcones, [12] pyrazolines [13], imines [14], flavones [15], pyrimidines [16], carboxamides [17], oxazines [18], epoxides [19], sulfonamides [20], acyl bromides [21], Tröger's bases [22], di-imines [23] and thiadiazoles [24]. Recently Thirunarayanan and Sekar was studied the spectral qsar correlations in the pyrazoline derivatives [25]. The correlation study of infrared and ^{13}C -NMR chemical shifts of aryl hydrazides with Hammett substituent constants and F and R parameters were established by Thirunarayanan et al., [26] Mayavel et al have studied the spectral correlations of infrared and NMR spectral frequencies of carbazole imines with Hammett substituent constants, F and R parameters [27]. Sathiyendiran et al. [28] have prepared some 2-oxopropyl diazenyl benzoic acids and studied the spectral correlation.

Within the above view, there is no reported for the spectral qsar studies of substituted quinoxalines in the past. Therefore the author have taken efforts to prepare some 5- and 6-substituted quinoxalines and recorded infrared and ^{13}C NMR spectra for the spectral correlations study.

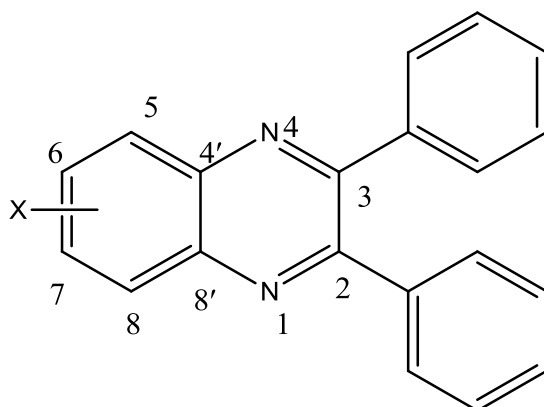
2. EXPERIMENTAL

2. 1. General

Sigma-Aldrich and Merck company chemicals and solvents used in this present study. The infrared spectra of all chalcones were recorded in SHIMADUZ Fourier Transform IR spectrophotometer using KBr discs. The ^{13}C NMR spectra of all compounds have been recorded in BRUKER AV 400 type spectrometer, using CDCl_3 as a solvent, 100 MHz for ^{13}C NMR spectra, taking TMS as standard.

2. 2. Synthesis of 5- and 6-substituted quinoxalines.

The 5- and 6-substituted quinoxalines were synthesized and the purities of the compounds were examined by literature method [1,29-31]. The general structure of the 5- and 6- substituted quinoxalines is shown in Fig. 1.



X= 6-H, 6-PhCO, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH₃, 5-CH₃, 6-CH₃, 6-NO₂

Fig. 1. General structure of substituted quinoxalines.

3. RESULTS AND DISCUSSION

In the present study, the authors have correlated the infrared and ^{13}C -NMR spectral frequencies with Hammett substituent constants, F and R parameters using single and multi-linear regression analysis. Present investigated compounds structure is shown is Fig. 1. It had symmetric structure. The substituents are in 5 and 6th position. With respect to $\text{C}_2=\text{N}_1$ and $\text{C}_8=\text{N}_1$, the substituents attached in 5 and 6th positions are considered as *meta*- and *para*-positions. Similarly, the $\text{C}_3=\text{N}_4$ and $\text{C}_4=\text{N}_4$, substituents attached in 5 and 6th positions are considered as *ortho*- and *meta*- positions. Within the considerations, the authors have performed the assigned spectral frequencies were correlated separately by the correlations performed with respect to $\text{C}_2=\text{N}_1$ and correlations performed with respect to $\text{C}_4=\text{N}_4$ systems

in the quinoxalines. The same trend was observed whether the substituents are attached in 8 and 7th positions.

3. 1. Infrared spectral correlation

The assigned the C=N stretches (cm^{-1}) of the present investigation substituted quinoxalines were tabulated in Table 1. These data were correlated with Hammett substituent constants, F and R parameters [12,14-28]. In this correlation, the Hammett equation was employed as,

Table 1. The infrared C=N stretches (cm^{-1}) and ^{13}C chemical shifts(ppm) of substituted quinoxalines.

Sl. No.	X	$\nu\text{C}=\text{N}$	$\delta\text{C}_2=\text{N}_1$	$\delta\text{C}_3=\text{N}_4$	$\delta\text{C}_4-\text{N}_4$	$\delta\text{C}_8-\text{N}_1$	$\delta\text{C}_{\text{ipso}}$
1	6-H	1567	153.49	154.75	141.24	139.10	129.95
2	6-COPh	1573	156.38	155.04	143.72	141.69	141.43
3	6-Br	1569	156.47	157.82	141.44	143.97	118.32
4	6-COOH	1563	157.64	156.64	141.73	144.11	135.60
5	6-Cl	1568	154.23	154.31	145.16	141.74	143.77
6	6-F	1571	155.04	156.72	143.09	140.62	166.53
7	6-OCH ₃	1552	153.08	156.74	144.37	139.32	162.23
8	5-CH ₃	1556	153.02	155.71	143.10	141.13	140.26
9	6-CH ₃	1557	153.18	156.41	143.22	141.63	139.32
10	6-NO ₂	1576	160.21	164.32	142.73	145.73	142.77

$$\nu = \rho\sigma + \nu_0 \quad \dots(1)$$

where ν_0 is the frequency for the parent member of the series.

The results of statistical analysis are tabulated in Table 2. From Table 2, the single parameter correlation of $\nu\text{C}=\text{N}$ *m*- and *p*- substituted quinoxalines gave satisfactory correlation coefficients with Hammett substituent constants, F and R parameters except fluoro substituent for σ_1 and R parameter. Similarly the single parameter correlation of these stretches of *o*- and *m*- substituted quinoxalines gave satisfactory correlation with Hammett σ , σ^+ , σ_1 constants and F parameters. The Hammett σ_R constants and R parameter were failing in correlations. All correlations gave positive ρ values. This meant that the normal substituent effect operates in all systems.

The failure in correlation was due to the inability of predicting the substituent effects on the frequencies along with the resonance conjugative structure as shown in Fig. 2.

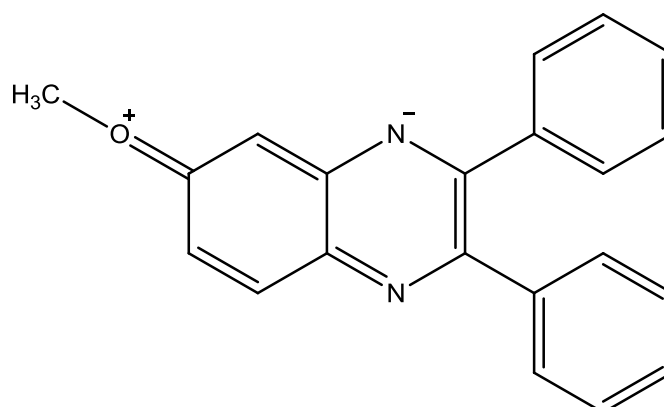


Fig. 2. The resonance-conjugative structure.

Table 2. Results of statistical analysis of IR and ^{13}C NMR spectral values of substituted quinoxalines with Hammett σ , σ^+ , σ_I , σ_R constants, F and R parameters.

Frequency	Constant	r	I	ρ	s	n	Correlated derivatives
Correlations performed with <i>p</i> -substitution pattern							
$\nu\text{C}=\text{N}$ (cm^{-1})	σ	0.917	1561.70	19.871	5.38	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.918	1594.41	14.100	4.15		
	σ_I	0.907	1558.27	23.022	6.21		
	σ_R	0.903	1567.00	16.012	8.02		
	F	0.906	1558.78	19.017	6.90		
	R	0.902	1566.01	7.449	8.42		
$\delta\text{C}_2=\text{N}_1$ (ppm)	σ	0.945	154.15	6.864	0.81	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.927	155.13	4.022	0.73		
	σ_I	0.907	153.35	6.655	1.77		
	σ_R	0.904	156.03	5.857	2.17		
	F	0.912	153.35	5.930	1.87		
	R	0.905	156.04	4.703	2.06		
$\delta\text{C}_3=\text{N}_4$ (ppm)	σ	0.905	156.07	4.983	2.24	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.904	156.80	2.372	2.27		
	σ_I	0.905	155.18	5.862	2.55		
	σ_R	0.831	157.42	4.231	2.85		
	F	0.901	155.14	5.372	2.58		
	R	0.825	157.03	2.513	2.89		
$\delta\text{C}_4-\text{N}_4$ (ppm)	σ	0.802	143.14	-0.849	1.31	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.836	143.04	-0.912	1.24		
	σ_I	0.890	142.84	0.547	1.33		
	σ_R	0.830	142.76	-1.890	1.28		
	F	0.810	142.94	0.173	1.34		
	R	0.841	142.66	-2.145	1.18		
$\delta\text{C}_8-\text{N}_1$ (ppm)	σ	0.980	141.11	5.190	1.34	10	6-H, 6-COPh, 6-Br,

	σ^+	0.969	141.85	2.907	1.58		6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ_I	0.905	140.72	4.251	1.93		
	σ_R	0.902	142.63	5.293	1.93		
	F	0.884	140.75	3.733	1.97		
	R	0.915	142.68	4.508	1.78		
δC_{ipso} (ppm)	σ	0.827	144.02	- 11.886	14.30	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.841	142.53	- 11.648	13.64		
	σ_I	0.822	138.52	12.087	14.52		
	σ_R	0.906	136.54	- 44.514	11.54		
	F	0.834	136.07	18.274	13.97		
	R	0.904	137.11	- 31.071	11.59		
Correlations performed with <i>m</i> -substitution pattern							
$\nu C=N$ (cm ⁻¹)	σ	0.907	1554.92	22.621	5.40	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.906	1562.60	10.908	6.86		
	σ_I	0.904	1558.54	22.871	5.92		
	σ_R	0.881	1567.48	17.534	7.54		
	F	0.901	1559.43	17.411	6.77		
	R	0.826	1566.37	7.391	8.17		
$\delta C_2=N_1$ (ppm)	σ	0.908	153.37	7.841	1.17	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.906	154.37	3.853	1.87		
	σ_I	0.907	153.22	7.029	1.73		
	σ_R	0.905	156.07	6.139	2.17		
	F	0.906	153.38	5.721	7.92		
	R	0.905	156.02	4.717	2.09		
$\delta C_3=N_4$ (ppm)	σ	0.963	155.22	6.703	2.32	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.904	156.19	2.741	2.75		
	σ_I	0.905	155.12	3.299	2.51		
	σ_R	0.830	157.41	4.370	2.86		
	F	0.905	153.45	6.357	2.58		
	R	0.825	155.07	2.532	2.91		
δC_4-N_4 (ppm)	σ	0.800	142.98	-0.033	1.33	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.808	142.91	0.268	1.33		
	σ_I	0.812	142.79	0.678	1.32		
	σ_R	0.813	142.72	-1.927	1.27		
	F	0.806	142.88	0.295	1.33		
	R	0.847	142.64	-2.138	1.17		
δC_8-N_1 (ppm)	σ	0.970	140.53	5.641	1.57	10	6-H, 6-COPh, 6-Br, 6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ^+	0.908	141.43	1.968	2.08		
	σ_I	0.905	140.48	4.947	1.84		
	σ_R	0.900	142.59	5.343	1.94		
	F	0.848	140.64	3.791	1.97		
	R	0.906	142.64	4.528	1.80		
δC_{ipso} (ppm)	σ	0.817	141.79	0.925	14.88	10	6-H, 6-COPh, 6-Br,

	σ^+	0.816	140.66	5.701	14.66	6-COOH, 6-Cl, 6-F, 6-OCH ₃ , 5-CH ₃ , 6-OCH ₃ , 6-NO ₂
	σ_I	0.819	138.78	11.102	14.59	
	σ_R	0.906	136.31	-43.86	11.57	
	F	0.836	135.73	18.978	13.84	
	R	0.907	137.07	13.062	11.60	

r = correlation coefficient; I = intercept; ρ = slope; s = standard deviation; n = number of correlated derivatives

3. 2. ¹³C NMR spectral correlation

The assigned the ¹³C NMR chemical shifts of substituted quinoxalines are presented in Table 1. These data are correlated with Hammett substituent constants, F and R parameters using single and multi-regression analysis [12,14-28]. In these correlations, the Hammett equation was taken in the form as,

$$\delta = \delta_0 + \rho\sigma \quad \dots (2)$$

where δ_0 is the chemical shift of the corresponding parent compound.

The results of statistical analyses are shown in Table 2. The correlations performed with respect to C₂=N₁ (*p*-substitution pattern), chemical shifts of $\delta_{C_2=N_1}$ (ppm) gave satisfactory correlation with Hammett substituent constants, F and R parameters. Hammett σ_R and F parameter gave satisfactory correlation except fluoro substituent. The $\delta_{C_3=N_4}$ (ppm) chemical shifts with Hammett σ and σ^+ constants gave satisfactory correlations except nitro substituent. The satisfactory correlations observed for Hammett σ_I and F parameters. The Hammett σ_R constant and R parameters were fails in correlations. All correlations gave positive ρ values. These mean that the normal substituent effect operates in all systems. The reason for the failure in the correlation was already stated and along with the resonance conjugative structure as shown in Fig. 2.

The single parameter correlation of $\delta_{C_4-N_4}$ (ppm) chemical shifts with Hammett substituent constants, F and R were failed. In these correlations, some of the negative ρ values obtained. This negative ρ values reduced correlations considerably. The reasons for this poor correlations were already stated and along with the resonance conjugative structure as shown in Fig. 2.

The single parameter correlation of $\delta_{C_8-N_1}$ (ppm) chemical shifts with Hammett substituent constants, F and R gave satisfactory r values. The F parameter was failed in the correlation. All correlations gave positive ρ values. The reason for the poor correlation of F parameter was already stated and along with the resonance conjugative structure as shown in Fig. 2.

The ipso carbon chemical shifts of the quinoxalines with Hammett σ_R constant and R parameters gave satisfactory correlations. The Hammett σ , σ^+ , σ_I constants and F parameter were fail in correlations. The inability of substituents along with conjugative structure as shown in Fig. 2. is explain the reasons for poor correlations.

The correlations performed with respect to C₄=N₃ (*m*- substitution pattern), the chemical shifts of $\delta_{C_2=N_1}$ (ppm) gave satisfactory correlation with Hammett substituent constants, F and R parameters. The $\delta_{C_3=N_4}$ (ppm) chemical shifts with Hammett σ , σ^+ and σ_I constants and F parameter constants gave satisfactory correlations. The Hammett σ_R constant and R parameters were failed in correlations. All correlations gave positive ρ values. These mean that the normal substituent effect operates in all systems. The reason for the failure in

the correlation was already stated and along with the resonance conjugative structure as shown in Fig. 2.

The chemical shifts δC_4-N_4 (ppm) of quinoxalines with Hammett substituent constants, F and R gave poor correlation. Some of correlations gave the negative ρ values obtained in this correlation. This negative ρ values reduced correlations considerably. The reasons for this poor correlations were already stated and along with the resonance conjugative structure as shown in Fig. 2.

The single parameter correlation of δC_8-N_1 (ppm) chemical shifts with Hammett substituent constants and F gave satisfactory r values. The R parameter was failed in the correlation. All correlations gave positive ρ values. The reason for the poor correlation of R parameter was already stated and along with the resonance conjugative structure shown in Fig. 2.

The ipso carbon chemical shifts of the quinoxalines with Hammett σ_I constant and R parameters gave satisfactory correlations. The Hammett σ , σ^+ , σ_R constants and F parameters were failed in correlations. Already stated the reason for the poor correlations and it is along with conjugative structure as shown in Fig. 2.

Some of the single parameters were failed in correlations with Hammett substituent constants, F and R parameters. While seeking multi-linear correlations with σ_I and σ_R constants or Swain Lupton's [32] F and R parameters gave satisfactory correlations for infrared and ^{13}C NMR spectral data of quinoxalines. The generated multi-regression analysis equations are shown in (3-26)

Correlations performed with *p*-substitution pattern

$$\nu C=N(\text{cm}^{-1}) = 1560.21(\pm 2.659) + 24.624(\pm 6.737)\sigma_I + 19.201(\pm 8.394)\sigma_R \quad \dots(3)$$

$$(R = 0.984, n = 10, P > 95 \%)$$

$$\nu C=N(\text{cm}^{-1}) = 1559.93(\pm 3.652) + 20.044(\pm 8.589)F + 9.360(\pm 0.817)R \quad \dots(4)$$

$$(R = 0.968, n = 10, P > 95 \%)$$

$$\delta C_2=N_1(\text{ppm}) = 154.03(\pm 0.588) + 7.222(\pm 1.490)\sigma_I + 6.739(\pm 1.857)\sigma_R \quad \dots(5)$$

$$(R = 0.990, n = 10, P > 95 \%)$$

$$\delta C_2=N_1(\text{ppm}) = 154.01(\pm 0.578) + 6.514(\pm 1.360)F + 5.324(\pm 1.268)R \quad \dots(6)$$

$$(R = 0.991, n = 10, P > 95 \%)$$

$$\delta C_3=N_4(\text{ppm}) = 155.69(\pm 1.310) + 6.283(\pm 3.319)\sigma_I + 5.045(\pm 2.142)\sigma_R \quad \dots(7)$$

$$(R = 0.963, n = 10, P > 95 \%)$$

$$\delta C_3=N_4(\text{ppm}) = 155.51(\pm 1.397) + 5.710(\pm 3.285)F + 3.063(\pm 0.306)R \quad \dots(8)$$

$$(R = 0.958, n = 10, P > 90 \%)$$

$$\delta C_4=N_4(\text{ppm}) = 142.66(\pm 0.722) + 0.394(\pm 0.183)\sigma_I - 1.838(\pm 0.221)\sigma_R \quad \dots(9)$$

$$(R = 0.930, n = 10, P > 90 \%)$$

$$\delta C_4=N_4(\text{ppm}) = 142.68(\pm 0.682) - 0.062(\pm 0.006)F - 2.152(\pm 0.127)R \quad \dots(10)$$

$$(R = 0.947, n = 10, P > 90 \%)$$

$$\delta C_8=N_1(\text{ppm}) = 141.324(\pm 0.831) + 4.750(\pm 2.107)\sigma_I + 5.907(\pm 2.623)\sigma_R \quad \dots(11)$$

$(R = 0.975, n = 10, P > 95 \%)$

$$\delta C_8=N_1(\text{ppm}) = 141.35(\pm 0.768) + 4.272(\pm 1.801)F + 4.915(\pm 1.685)R \quad \dots(12)$$

$(R = 0.980, n = 10, P > 95 \%)$

$$\delta C_{\text{ipso}}(\text{ppm}) = 134.19(\pm 6.400) + 8.501(\pm 1.621)\sigma_I - 42.971(\pm 20.204)\sigma_R \quad \dots(13)$$

$(R = 0.964, n = 10, P > 95 \%)$

$$\delta C_{\text{ipso}}(\text{ppm}) = 133.42(\pm 6.258) + 15.023(\pm 1.472)F - 29.343(\pm 13.708)R \quad \dots(14)$$

$(R = 0.968, n = 10, P > 95 \%)$

Correlations performed with *m*-substitution pattern

$$\nu C=N(\text{cm}^{-1}) = 1560.79(\pm 2.527) + 23.558(\pm 6.304)\sigma_I + 18.850(\pm 7.737)\sigma_R \quad \dots(15)$$

$(R = 0.985, n = 10, P > 95 \%)$

$$\nu C=N(\text{cm}^{-1}) = 1549.43(\pm 3.496) + 17.414(\pm 8.345)F + 14.321(\pm 6.173)R \quad \dots(16)$$

$(R = 0.968, n = 10, P > 95 \%)$

$$\delta C_2=N_1(\text{ppm}) = 154.00(\pm 0.603) + 7.264(\pm 1.505)\sigma_I + 6.532(\pm 1.847)\sigma_R \quad \dots(17)$$

$(R = 0.991, n = 10, P > 95 \%)$

$$\delta C_2=N_1(\text{ppm}) = 154.01(\pm 0.582) + 6.437(\pm 1.354)F + 5.482(\pm 1.297)R \quad \dots(18)$$

$(R = 0.991, n = 10, P > 95 \%)$

$$\delta C_3=N_4(\text{ppm}) = 155.01(\pm 1.270) + 6.229(\pm 3.400)\sigma_I + 4.720(\pm 0.407)\sigma_R \quad \dots(19)$$

$(R = 0.964, n = 10, P > 95 \%)$

$$\delta C_3=N_4(\text{ppm}) = 155.44(\pm 1.372) + 5.766(\pm 3.189)F + 3.223(\pm 0.132)R \quad \dots(20)$$

$(R = 0.960, n = 10, P > 90 \%)$

$$\delta C_4=N_4(\text{ppm}) = 142.57(\pm 0.733) + 0.563(\pm 0.183)\sigma_I - 1.894(\pm 0.224)\sigma_R \quad \dots(21)$$

$(R = 0.932, n = 10, P > 90 \%)$

$$\delta C_4=N_4(\text{ppm}) = 142.63(\pm 0.671) + 0.016(\pm 0.005)F - 2.136(\pm 0.149)R \quad \dots(22)$$

$(R = 0.947, n = 10, P > 90 \%)$

$$\delta C_8=N_1(\text{ppm}) = 141.13(\pm 0.815) + 5.149(\pm 2.033)\sigma_I + 5.622(\pm 0.246)\sigma_R \quad \dots(23)$$

$(R = 0.978, n = 10, P > 95 \%)$

$$\delta C_8=N_1(\text{ppm}) = 141.23(\pm 0.725) + 4.453(\pm 1.696)F + 5.061(\pm 1.624)R \quad \dots(24)$$

$(R = 0.982, n = 10, P > 95 \%)$

$$\delta C_{\text{ipso}}(\text{ppm}) = 133.60(\pm 6.550) + 9.543(\pm 1.634)\sigma_I - 43.352(\pm 2.062)\sigma_R \quad \dots(25)$$

$(R = 0.964, n = 10, P > 95 \%)$

$$\delta C_{\text{ipso}}(\text{ppm}) = 132.95(\pm 6.148) + 15.156(\pm 1.429)F - 29.249(\pm 13.623)R \quad \dots(26)$$

$(R = 0.968, n = 10, P > 95 \%)$

4. CONCLUSIONS

A series containing ten substituted 5- and 6- substituted quinoxaline derivatives have been synthesized and examined their purities by literature method. The infrared and ^{13}C NMR spectral frequencies of C=N, C-N and ipso carbons of the quinoxalines were assigned and correlated based on *m*- and *p*- substituted system with Hammett substituent constants, F and R parameters using single and multi-regression analysis. From the results of statistical analyses, most of the single parameter correlations and all multi- correlations gave satisfactory correlation coefficients.

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