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Synthesis, characterization and spectral correlations in substituted styryl 6-methyl-2-naphthyl ketones

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Thirteen substituted styryl 6-methyl-2-naphthyl ketones [(2E)-1-(6-methyl-2-naphthyl)-3-phenyl-2-propen-1-ones] are synthesized using eco-friendly benign stereo selective crossed - aldol condensation reaction assisted by silica-sulphuric acid reagent under solvent-free conditions. The yield of chalcones is more than 90%. No decrease in the yield is observed during synthesis and demonstrating that silica-sulphuric acid can be reused in crossed-aldol condensation reaction without environmental discharge. They have been characterized by their physical constants, micro analysis, infrared, NMR and mass spectral data. These spectral data are subjected to correlate various Hammett substituent constants with single and multiparameter correlation equations. From the results of statistical analysis, the influence of electronic effects of substituents on the spectral data of carbonyl group, vinyl proton and carbons of the ketones are explained.

Keywords: Styrylketones, aldol condensation, silica-sulphuric acid, chalcones

In recent years, chemists are paying more interest in the application of solvent free methods[1] in organic reactions like Claisen-Schmidt[2], Knovenogal[3], Aldol[4] and Crossed-aldol[5] for synthesis of carbonyl compounds due to the operational simplicity, easier work-up, better yield and eco-friendly nature. Among these reactions aldol condensation is useful for the formation of carbon-carbon bond in many kinds of carbonyl compounds[6]. The methylene unit of chalcones derived from cyclic or acyclic ketones are found in many naturally occurring compounds and they are useful for the synthesis of pyrimidine derivatives[7]. The basic skeleton of chalcones is widely figured in natural products, are known to have multipronged activity[8]. Many of the chalcones are used as agrochemicals and drugs[9]. Condensation of ketones with aldehydes is of special interest and crossed-aldol condensation is an effective pathway for those preparations. But traditional acid-base catalyzed reactions suffer from the reverse reaction[10] and self condensation of starting molecules[11].

Many reagents and co-ordination complexes of Mn(II), Fe(II), Co(II), Ni(II), Cu(II) and Zn (II) ions with various ligands have been employed for aldol condensation[12]. Metal salts of Cp_2ZrH_2 are used for condensation of cycloalkanones[13] KF-Al_2O_3 and bis (*p*-methoxy phenyl) tellurides have been used for crossed condensation under microwave irradiation[14]. Anhydrous $RuCl_3$ and $TiCl_3$ (SO_3CF_3) have also been applied for aldol condensation reactions under solvent free conditions[15]. Now more attention has been paid to synthesis of acyclic and cyclic chalcones by chemists and scientists[16]. Kalluraya[17] *et al.* reported to obtain 60-70% yield of sydnone chalcones under solvent free condition by aldol condensation reaction by grinding of ketones and aldehydes with sodium hydroxide. Hassan[18] *et al.* synthesized various *2E*-3-aryl-1-heteroarylprop-2-en-1-ones by eco-friendly condensation reaction in sodium hydroxide-water heterogeneous phase reaction medium. Silica-sulphuric acid is used as a versatile and stable solid acid catalyst for organic synthesis. An efficient and selective method for condensation of 6-methyl-2-acetonaphthones with various *m*- and *p*-substituted benzaldehydes under solvent free conditions using silica-sulphuric acid as a reagent in an oven to yields the respective *E*-2-propen-1-ones is reported. The promoting effect of silica-sulphuric acid in this reaction has shown good performance and its catalytic activity is proved by obtaining higher percentage of yields. The product was isolated and the remaining catalyst was washed and reused with fresh substrate for further reactions. No decrease in the yield was observed, demonstrating that silica-sulphuric acid can be reused in crossed-aldol condensation reaction without environmental discharge.

Experimental Section

Materials and Methods

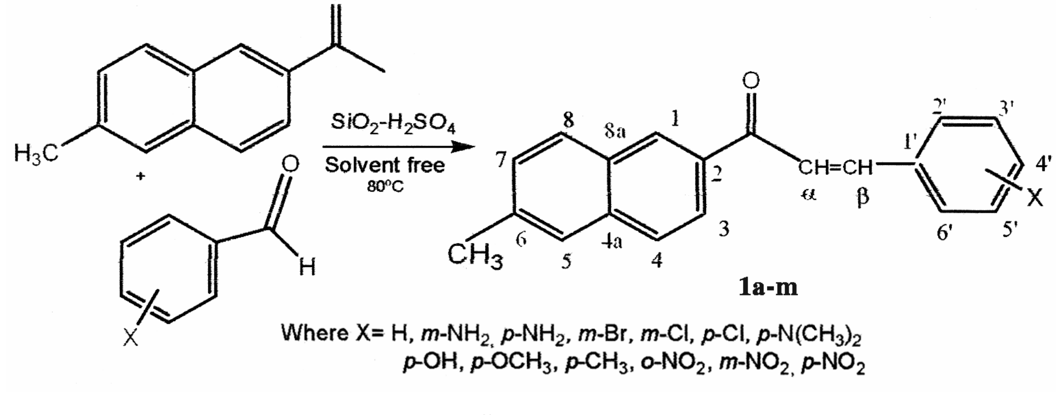
All chemicals and analytical grade solvents were purchased from E-Merck chemical company. Melting points of all chalcones were determined in open glass capillaries on Mettler FP51 melting point apparatus and are uncorrected. Infrared spectra (KBr) were recorded on a Perkin Elmer-Fourier transform spectrophotometer. The nuclear magnetic resonance spectra, both ^{1}H and ^{13}C, of chalcones were recorded using UNITYPLUS-300 KIBSIPS 300 MHz spectrometer. Electron impact (EI, 70 eV) and chemical ionization (CI) mass spectra were recorded with a Finnigan MAT 95S spectrometer. Micro analyses of all chalcones were performed in Perkin-Elmer 240C Analyzer.

General procedure for synthesis of substituted styryl 6-methyl-2-naphthyl ketones:

6-Methyl-2-naphthyl ketones (2 mmole), *m*-and *p*-substituted benzaldehydes (2.2 mmole) and silica-sulphuric acid (1.5 g equal to 4 mmole of H$^+$) were mixed thoroughly, placed in a glass tube and capped (**Scheme I**). The mixture was heated in an oven at 80°C for 2-3.5 hr. After complete conversion of the ketones as monitored by TLC, the mixture was cooled to room temperature. Dichloromethane (20-30 mL) was added and warmed for 3-5 minutes. The reagent was removed by filtration. The filtrate was concentrated and the solid residue was recrystallised from ethanol to afford the pure products as pale yellow glittering solids **1a-m** (ref. 19). The catalyst was recycled by washing the solid reagent with ethyl acetate (20 mL) followed by drying in an oven at 50°C for two hr and it is reused for another reaction run. Based on Hays and Timmons[20,21] infrared carbonyl-stretching frequencies of *s-cis* and *s-trans* conformers are assigned. The NMR chemical shifts (ppm) of ethylene α,β protons and carbons are assigned based on reported in earlier literature values[22-27] of the compound **1a**. The characterization data of all chalcones are summarized in **Table I**.

Substituent effects

Correlation analysis involves the prediction of ground state molecular equilibrations[29] of organic substrates such as *s-cis* and *s-trans* isomers of alkenes, alkynes, benzoylbromides, benzoylchlorides, diphenylamine[30] styrenes and α,β-unsaturated ketones from spectral data. Their use in structure parameter correlations has now become popular for studying transition state study of reaction mechanisms[31] biological activities and normal coordinate analysis[32]. Dhami and Stothers[33] have extensively studied the ^{1}H NMR spectra of a large number of acetophenones and styrenes with a view to establish the validity of the additivity of substituent effects in aromatic shieldings, first observed by Lauterber[34]. Savin and coworkers[35] obtained the NMR spectra of unsaturated ketones of the type RC_6H_4-CH=CH-$COCMe_3$ and sought Hammett correlations for the ethylenic protons. Solcaniova and coworkers[36] have measured ^{1}H and ^{13}C NMR spectra of substituted phenyl styrenes and substituted styryl phenyls and obtained good Hammett correlations for the olefinic protons and carbons. Nowadays scientists[37] have shown greater interest to correlate the group frequencies of spectral data with Hammett substituent constants to explain the substituent effect of organic compounds. Recently Sung and Nadar[38] investigate elaborately the single and multi substituent effects by spectral data of biphenyl and 9*H*-Fluorenyl chalcones. Within the above view there is no information available in the



Where X= H, *m*-NH$_2$, *p*-NH$_2$, *m*-Br, *m*-Cl, *p*-Cl, *p*-N(CH$_3$)$_2$ *p*-OH, *p*-OCH$_3$, *p*-CH$_3$, *o*-NO$_2$, *m*-NO$_2$, *p*-NO$_2$

Scheme I

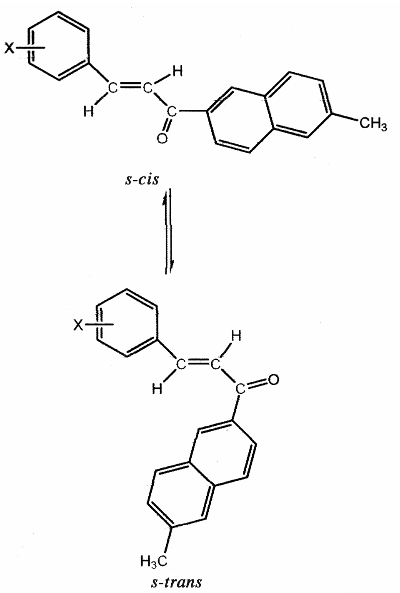
Table I — Physical constants, microanalysis and mass spectral data of substituted styryl 6-methyl-2-naphthyl ketones

Entry	Mol. formula	Mol. weight	Yield (%)	m.p. °C	Found %(Calcd) C	H	N	Mass m/z
1a	$C_{20}H_{16}O$	272.34	96	123-124 124 (ref. 28)	—	—	—	272[M$^+$], 169,141, 131, 127, 103, 77
1b	$C_{20}H_{17}NO_2$	287.35	91	106-107	83.42 (83.59	5.90 5.96	4.81 4.87)	287[M$^+$], 271, 169, 146, 141, 127, 118
1c	$C_{20}H_{17}NO_2$	287.35	93	95-96	83.54 (83.59	5.96 5.96	4.85 4.87)	287[M$^+$], 286, 271, 169, 146, 141, 127, 118, 103
1d	$C_{20}H_{15}BrO$	351.23	94	82-83	68.30 (68.30	4.25 4.30)	—	351[M$^+$], 208, 196, 180, 141, 65
1e	$C_{20}H_{15}ClO$	306.78	92	146-47	78.25 (78.30	4.86 4.93)	—	306[M$^+$], 268, 168, 137, 103, 65.
1f	$C_{20}H_{15}ClO$	306.78	95	154-55	78.28 (78.30	4.90 4.93)	—	306[M$^+$], 280, 168, 140, 137, 128, 103, 77, 65.
1g	$C_{22}H_{21}NO$	315.40	94	73-74	83.72 (83.78	6.61 6.71)	4.39 4.44)	315[M$^+$], 271, 168, 146, 142, 140, 128, 91, 77
1h	$C_{20}H_{16}O_2$	228.33	91	80-81	83.29 (83.31	5.48 5.50)	—	288[M$^+$], 271, 199, 141, 128, 119, 107, 103, 91
1i	$C_{21}H_{18}O_2$	302.36	95	131-33	83.36 (83.42	5.72 6.00)	—	302[M$^+$], 271,168, 140, 136, 128, 105, 91, 77, 65
1j	$C_{21}H_{18}O$	286.36	96	109-10	88.03 (88.08	6.29 6.34)	—	286[M$^+$], 271, 168, 140, 128, 117, 103, 91, 77, 65
1k	$C_{20}H_{15}NO_3$	317.33	92	106-07	75.63 (75.70	4.62 4.76	4.09 4.41)	317[M$^+$], 168, 142, 126, 116, 103, 91
1l	$C_{20}H_{15}NO_3$	317.33	94	134-35	75.65 (75.70	4.70 4.76	4.32 4.41)	317[M$^+$], 168, 142, 126, 116, 103, 91, 77, 65.
1m	$C_{20}H_{15}NO_3$	317.33	96	177-78	75.68 (75.70	4.72 4.76	4.39 4.41)	317[M$^+$], 168, 142, 126, 116, 103, 91, 77, 65

literature in the past with substituted styryl 6-methyl-2-naphthyl ketones. Hence thirteen chalcones of the above type using silica-sulphuric acid technique are synthesized and the substituent effects of above compounds are investigated from infrared and NMR spectra were made.

Substituent effects from infrared spectra

The carbonyl stretching frequencies (cm^{-1}) of *s-cis* and *s-trans* isomers of present study are presented in **Table II** and the corresponding conformers are shown in I. The infrared spectra were all recorded on the KBr disc in order to avoid the shoulder formation[39] on carbonyl doublets. The *s-cis* conformers exhibit higher frequencies than the *s-trans* conformers due to the bulkier naphthalene group causes greater strain and they enhance the higher absorption of carbonyl group of *s-cis* isomer (1651-1680 cm^{-1}) than the *s-trans* isomer (1608-1633 cm^{-1}). These frequencies are separately analyzed through various Hammett sigma[40] constants. From the statistical analysis, fair degree of correlation obtained[r=0.945, I=1660.53, ρ=1.76, s=0.32, n=13] with Hammett sigma constants in *s-cis* conformers. Hammett σ_I constants in *s-trans* isomers produce a fair correlation with carbonyl



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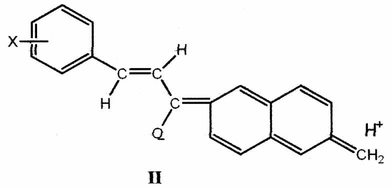


II

Table II—Spectral data of substituted styryl 6-methyl -2-naphthyl ketones

Entry	IR ν(cm^{-1})				^{1}H NMR δ (ppm)				
	CO (*s-cis*)	CO (*s-trans*)	CH=CH	Subst. in Ph. ring	d,1H, α	d,1H, β	m, Ar-H	Subst. in Ph. ring	s, 3H, -CH_3 (Nap)
1a	1658	1616	985	—	8.063	8.107	7.369-7.844 (11H)	—	2.454
1b	1661	1616	1018	3532(-NH_2)	8.058	8.093	7.155-7.876 (10H)	4.430 (s,2H, NH_2)	2.637
1c	1651	1613	974	3527(-NH_2)	8.082	8.992	7.760-7.940 (10H)	4.187 (s,2H, NH_2)	2.543
1d	1666	1625	1013	—	8.040	8.090	7.342-7.892 (10H)	—	2.695
1e	1660	1627	1029	—	8.056	8.100	7.320-7.843 (10H)	—	2.864
1f	1663	1625	998	—	8.049	8.091	7.129-8.000 (10H)		2.395
1g	1651	1608	984	—	8.051	8.093	6.830-7.880 (10H)	2.078 (s,6H, $N(CH_3)_2$)	2.621
1h	1656	1625	1014	3541(-OH)	7.974	8.021	6.893-7.789 (10H)	4.621 (s,1H, OH)	2.287
1i	1655	1619	1005	—	8.051	8.093	7.012-7.874 (10H)	3.655 (s,3H, OCH_3)	2.721
1j	1655	1607	973	—	8.056	8.098	7.282-7.898 (10H)	2.679 (s,3H, CH_3)	2.366
1k	1680	1633	1014	—	8.072	8.073	7.575-8.045 (10H)	—	2.721
1l	1674	1622	1024	—	8.082	8.154	7.354-8.042 (10H)	—	2.593
1m	1677	1624	1020	—	8.091	8.291	7.370-8.092 (10H)	—	2.630

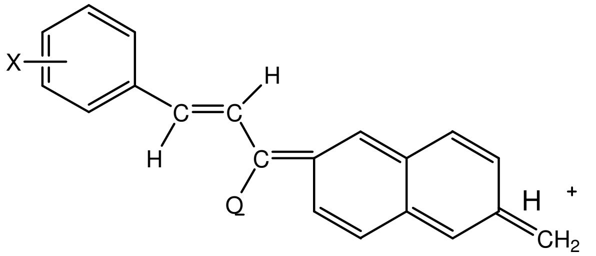
frequencies[r=0.901, I=1611.93, ρ=2.55, s=0.42, n=13]. Remaining σ^+, σ_I and σ_R constants failed for producing a correlation. The reason for the failed correlation is the conjugation between the C=O and the -CH=CH- parts are important due to non-co planarity arising out of non bonded repulsion between naphthalene and styryl parts in the systems and the cross conjugation of methyl substituent in sixth position of naphthyl ring as shown in II. Due to the extended conjugation by the naphthyl ring reduces the correlation on carbonyl frequencies. In view of the inability of some σ constants to produce individually satisfactory correlations, it was thought worthwhile to seek multiple correlations involving either σ_I and σ_R constants or F and R parameters. This may be treated as exceptional and by and large it is to be realized that the collective participation of either σ_I and σ_R constants or F and R parameters is more dependent than that of any single parameter role to predict the substituent effects. The correlation equations are:

$$\nu C{=}O(s\text{-}cis)\ (\text{cm}^{-1}) = (1658.004 \pm 3.149) + (23.278 \pm 6.240)\ F + (10.918 \pm 2.547)\ R \quad \ldots (1)$$

$$(R = 0.914, n=13, P > 95\%)$$

$$\nu C{=}O(s\text{-}trans)(\text{cm}^{-1}) = (1611.403 \pm 2.458) + (24.252 \pm 3.214)\ \sigma_I - (1.576 \pm 0.257)\ \sigma_R \quad \ldots (2)$$

$$(R = 0.908, n=13, P > 92\%)$$



II

$$\nu C{=}O(s\text{-}trans)\ (\text{cm}^{-1}) = (1612.521 \pm 3.648) + (20.324 \pm 3.254)\ F + (1.364 \pm 0.218)R \quad \ldots (3)$$

$$(R = 0.904, n=13, P > 92\%)$$

Substituent effects from NMR Spectra

^{1}H NMR Spectra

The ^{1}H NMR spectral signals of ethylenic protons in all chalcones investigated are assigned. The observation that H_α protons appear at higher field than that of H_β protons makes the subject very interesting. This may possibly due to the polarization of C=C double bond in the system being predominantly caused by the carbonyl group so as to make electron density greater at α position than that of β position. The chemical shifts of H_α protons are at higher field than those of H_β protons in all chalcones. The ethylenic proton signals give an AB pattern and the β protons doublet in most cases is well separated from the signals of the aromatic protons. The chemical shifts of α, β protons are given in **Table II**. All the attempted correlations involving substituent parameters gave only positive ρ values. This shows normal substituent effects operate in all the chalcones. The chemical shifts observed for H_α and the H_β protons in the present investigation are correlated satisfactorily with Hammett sigma[40] and σ^+ constants. In some cases correlation of Hα with σ_R values are well correlated (r= 0.993). H_β chemical shifts with σ_I and σ_R are not correlated well. This is due to the fact that values are incapable of predicting chemical shifts individually and domination of cross conjugation between carbonyl group and methyl group in naphthyl ring. The correlation equations (4-8) are:

$$H_{\alpha(ppm)} = (8.045 \pm 0.023) + (0.042 \pm 0.012)\sigma \quad \ldots (4)$$
(r=0.936, s=0.025, n=13)

$$H_{\alpha(ppm)} = (8.052 \pm 0.126) + (0.026 \pm 0.010)\sigma^+ \quad \ldots (5)$$
(r=0.924, s=0.055, n=13)

$$H_{\alpha(ppm)} = (8.057 \pm 0.021) + (0.064 \pm 0.015)\sigma_R \quad \ldots (6)$$
(r=0.993, s=0.021, n=13)

$$H_{\beta(ppm)} = (8.097 \pm 0.048) + (0.035 \pm 0.001)\sigma \quad \ldots (7)$$
(r=0.930, s=0.065 n=13)

$$H_{\beta(ppm)} = (8.099 \pm 0.043) + (0.021 \pm 0.004)\sigma \quad \ldots (8)$$
(r=0.912, s=0.021 n=13)

The multiple correlation involving σ_I and $\sigma_{R\ \mathrm{or}}$ F and R values with these chemical shifts for these ketones are successful and they generated the equations (9-11)are:

$$H_{\alpha(ppm)} = (8.051 \pm 0.016) + (0.017 \pm 0.036)\sigma_I + (0.057 \pm 0.031)\sigma_R \quad \ldots (9)$$
(R = 0.999, n=13, P > 99%)

$$H_{\alpha(ppm)} = (8.086 \pm 0.020) - (0.601 \pm 0.041)F + (0.541 \pm 0.025)R \quad \ldots (10)$$
(R = 0.918, n=13, P > 90%)

$$H_{\beta(ppm)} = (8.097 \pm 0.039) + (0.015 \pm 0.003)\sigma_I + (0.046 \pm 0.001)\sigma_R \quad \ldots (11)$$
(R = 0.913, n=13, P > 92%)

^{13}C NMR Spectra

From ^{13}C NMR spectra the observed ^{13}C chemical shifts of C_α and the C_β carbons are presented in **Table III**. These chemical shifts are correlated with various Hammett substituent constants. From the results of statistical analysis of substituent effects on C_α and C_β carbons produce a fair degree of correlation with Hammett sigma[40] constants except σ_I and σ_R. The degree of transmission of electronic effects is found to be higher with C_α carbon (r=0.974 for σ) than C_β carbon (r=0.900 for σ). In both cases the resonance effect of the substituents fails to produce the correlation on vinyl carbons. Because, the phenyl ring and the vinyl part are not co-planar due to carbon-carbon single bond rotation, that the deviations vary with the type of substitution. The successful correlation equations (12-15) are:

$$C_{\alpha(ppm)} = (120.451 \pm 0.012) + (1.867 \pm 0.010)\sigma \quad \ldots (12)$$
(r=0.974, s=0.288, n=13)

$$C_{\alpha(ppm)} = (120.798 \pm 0.152) + (1.160 \pm 0.110)\sigma^+ \quad \ldots (13)$$
(r=0.964, s=0.387, n=13)

$$C_{\alpha(ppm)} = (119.567 \pm 0.241) + (3.319 \pm 0.254)\sigma_I \quad \ldots (14)$$
(r=0.913, s=0.581, n=13)

$$C_{\beta(ppm)} = (1143.167 \pm 1.265) + (1.969 \pm 0.066)\sigma \quad \ldots (15)$$
(r=0.900, s=1.275, n=13)

Uniformly, σ_I and σ_R parameters or F and R values adequately explain the substituent effects in all chalcones evidenced from the multi correlation equations (16-19).

$$C_{\alpha(ppm)} = (119.721 \pm 0.340) + (3.047 \pm 0.124)\sigma_I + (0.485 \pm 0.065)\sigma_R \quad \ldots (16)$$
(R = 0.918, n=13, P > 90%)

$$C_{\alpha(ppm)} = (120.777 \pm 0.395) + (2.232 \pm 0.783)F + (1.181 \pm 0.496)R \quad \ldots (17)$$
(R = 0.936, n=13, P > 90%)

$$C_{\beta(ppm)} = (143.734 \pm 0.655) - (0.308 \pm 1.447)\sigma_I + (2.819 \pm 1.257)\sigma_R \quad \ldots (18)$$
(R = 0.905, n=13, P > 90%)

$$C_{\beta(ppm)} = (143.577 \pm 0.989) + (0.315 \pm 1.961)F + (1.1292 \pm .214)R \quad \ldots (19)$$
(R = 0.911, n=13, P > 90%).

Conclusion

This synthetic methodology is very efficient and selective protocol for crossed-aldol condensation of 6-methyl-2-naphthyl ketones and aldehydes to produce high yield of 6-methyl-2-naphthyl chalcones in the presence of a reusable and environmentally beginning reaction catalyst silica-sulphuric acid. Operative simplicity, easy procedure, better yield including washing the mixture followed by evaporation of the solvent are other advantages of this method. In correlation analyses of infrared spectral data, σ

Table III— ^{13}C NMR of substituted styryl 6-methyl-2-naphthyl ketones

Entry	C_α	C_β	C=O	C_1	C_2	C_3	C_4	C_5	C_6
1a	120.488	142.821	192.047	128.634	132.996	125.338	127.398	126.417	136.921
1b	120.628	144.147	190.210	128.424	133.296	125.058	127.698	126.821	136.381
1c	118.972	141.887	188.620	128.214	133.592	125.076	127.075	125.948	136.994
1d	121.421	141.979	191.254	128.574	133.196	125.903	127.621	126.032	136.371
1e	121.686	141.015	191.784	128.230	133.731	125.739	127.695	126.752	137.839
1f	120.912	142.958	191.560	128.304	133.498	125.142	127.964	125.916	136.904
1g	119.230	141.530	189.524	128.530	132.949	125.800	127.699	126.763	136.953
1h	119.900	143.210	191.200	127.992	132.875	125.713	126.751	126.405	136.990
1i	120.143	144.669	190.201	127.530	134.286	125.061	127.632	126.703	137.530
1j	119.524	144.376	198.621	128.643	134.831	124.721	127.996	126.596	137.821
1k	121.421	144.126	192.254	128.407	134.201	125.630	126.841	126.472	137.439
1l	123.943	144.669	193.251	128.703	135.325	124.443	126.998	126.754	137.669
1m	121.815	144.794	193.872	128.329	133.926	124.016	127.349	126.024	137.365

Entry	C_7	C_8	C_{4a}	C_{8a}	CH_3	C_1’	C_2’	C_3’	C_4’
1a	128.290	127.996	132.648	133.491	23.106	135.632	126.814	128.381	126.699
1b	128.309	127.295	132.399	133.612	24.323	135.699	113.268	148.381	116.699
1c	128.941	127.929	132.476	133.697	24.017	125.359	127.926	118.381	146.629
1d	128.941	127.219	132.302	133.571	22.998	137.398	128.907	124.381	131.899
1e	128.602	127.929	132.403	133.594	26.948	136.573	126.754	134.331	128.011
1f	128.697	127.979	132.499	133.603	26.007	133.054	126.991	129.971	134.365
1g	128.802	128.694	132.742	133.901	25.721	125.675	127.621	115.064	148.346
1h	128.041	128.677	132.122	133.002	23.621	127.887	127.682	115.734	156.994
1i	128.769	128.883	132.538	133.497	25.450	127.648	127.399	114.622	159.924
1j	128.804	128.691	132.946	133.753	24.963	132.148	126.453	130.101	137.597
1k	127.998	128.883	132.964	133.795	22.598	129.052	146.014	121.441	128.995
1l	129.532	128.964	132.064	133.091	22.830	136.014	122.364	147.992	130.967
1m	128.871	128.906	132.547	133.226	23.001	141.365	127.995	122.001	147.599

Entry	$C_{5'}$	$C_{6'}$	Subst. in Ph ring
1a	128.381	126.814	—
1b	129.587	116.618	—
1c	118.381	127.926	—
1d	129.991	124.969	—
1e	129.971	142.766	—
1f	129.971	126.991	—
1g	115.064	127.621	41.043 [$N(CH_3)_2$]
1h	115.743	127.682	—
1i	114.622	127.399	54.325 [OCH_3]
1j	130.101	126.453	24.963 (CH_3)
1k	135.821	127.696	—
1l	130.967	133.365	—
1m	122.001	127.995	—

constants produce a fair correlation with carbonyl absorption frequencies in both conformers of all chalcones. Nuclear magnetic resonance spectral data correlation, H_β chemical shifts correlated with σ^+ constants are well correlated than H_α. Other Hammett constants produce a fair correlation except σ_I constant. A satisfactory correlation is obtained by correlation of C_α and C_β chemical shifts with Hammett σ and σ^+ substituent constants, failure with σ_R values. Overall collective multi correlation of σ_I and σ_R parameters or F and R values with carbonyl frequencies, hydrogen and carbon chemical shifts of vinyl moiety are produce satisfactory correlation.

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