**Substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one**.

(E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one and its *p*-substituted compounds were prepared by the following procedure67SP.

The mixture of the calculated amount of the pure 2-acetylfuran (0.55g ~ 0.005 moles) in cold ethanol and 10% solution of sodium hydroxide (catalytic amount) was cooled in a water bath to 0o C. To this mixture pure benzaldehyde (0.583 g ~ 0.0055 moles) in cold ethanol was added drop by drop for 30 minutes. The reaction mixture stirred for 2 hours. Then it was kept in the refrigerator for overnight. The precipitated solid was collected and recrystallized using ethanol-chloroform (10:1) mixture.



All the substituted compounds were prepared by using the above procedure.

**Characterization**

All the compounds were characterized as (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one and its derivatives by 1H and 13C NMR spectral techniques. All 1H and 13C NMR spectra were obtained on a BRUKER AV 400 MHz spectrometer. Chemical shifts of 1H were measured with the central peak of CDCl3 at δ 7.259 as the internal reference, while those of 13C were measured with the central peak of CDCl3 at δ 77.54 as the internal reference.



In 1H NMR spectra of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones whose signals assignment were not difficult and all signals well separated from each other. The -CH- proton of C11 carbon atom is expected to downfield than -CH- proton of C9 carbon atom. The -CH- proton of C10 is well separated from all other protons signals, hence it’s assignment is not difficult. Two ethylenic protons C6 and C5 carbon atoms are well separated from each other. The α-ethylenic proton is expected to be downfield shift since it is proximity to the carbonyl group. Assignment of the signals was based on splitting pattern and peak integration ratio. 1H NMR spectra of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones are given in Fig’s ( ).

**1H NMR spectra of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones are given below.**

1. **(E)-1-(furan-2-yl)-3-(4’ -N,N dimethylaminophenyl)prop-2-ene-1-one:**

**δ :** 3.043 (s,6H), 6.562 (d,d,1H), 6.6909 (d,2H), 7.256 (d,1H), 7.262 (d,1H),

7.554 (d,2H), 7.616 (m,1H), 7.856 (d,1H).

1. **(E)-1-(furan-2-yl)-3-(4’ -methylphenyl)prop-2-ene-1-one:**

**δ:**

1. **(E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one:**

**δ:** 6.600 (d,d,1H), 7.336 9d,1H), 7.421 (m.2H), 7.423 (d,1H), 7.456(d,1H), 7.655(m,2H),

**7.**657(m,1H), 7.885(d,1H).

1. **(E)-1-(furan-2-yl)-3-(4’ -chlorophenyl)prop-2-ene-1-one:**

**δ:** 6.606(d,d,1H), 7.339(d,1H), 7.394(d,2H), 7.425(d,1H), 7.584(d,1H), 7.584(d,2H),

7.658(m,1H), 7.822(d,1H).

5. **(E)-1-(furan-2-yl)-3-(4’ -fluorophenyl)prop-2-ene-1-one:**

**δ:** 6.599 (d,d,1H), 7.107(m,2H), 7.329(d,1H), 7.380(d,1H), 7.642(m,2H), 7.650(m,1H),

7.837(d,1H).

6. **(E)-1-(furan-2-yl)-3-(4’ -oxophenyl)prop-2-ene-1-one:**

**δ:**

**Assignment of 13C NMR signals**

13C NMR signals were assigned for various carbons were based on the

1. Chemical shift exhibited by the signals
2. Relative signal intensity,
3. Empirical additivity rules.



Fig. ()

where X is the substituents viz. *p*-NMe2, *p*-Me, H, *p*-Cl, *p*-F, *p*-CHO. 13C NMR spectra of *para*-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones are given in Fig. (). The proton noise decoupled spectrum of parent compound contains 11 signals corresponding to 11 different carbon atoms. In all the spectra, carbonyl carbon signal was readily recognized from its low intensity and also well separated from other signals to the downfield extreme, since its assignment was not difficult.

Two more low-intensity peaks were readily assigned for C8 and C4 carbon atoms. Due to nearby oxygen atoms in the ring the downfield signal at 153.73 ppm was assigned for C8 carbon atom. The upfield signal at 134.75 ppm was assigned for C4 carbon atom.

There are remaining eight signals for eight carbon atoms in which, six signals appeared almost same intensity other two signals appeared twice in intensity. This is due to the number of protons attached to the sp2 carbon atoms. The two high-intensity signals were readily assigned for aromatic carbon C3,3’ and C2,2’ atoms. This is due to the styrene as substituent since the upfield signal is 128.54 ppm was assigned for (*ortho*) C2,2’ carbon atom and next downfield signal at 128.96 ppm was assigned for (*meta*) C3,3’ carbon atom.

There are remaining six same intensity signals in which most downfield extreme signals at 146.53 ppm was assigned to C11 carbon atom of furon ring because it is directly attached to the oxygen atom.

Among the remaining downfield signals of the two upfield signals were assigned for C9 and C10 carbon atoms. The signal at 117.52 ppm was assigned for C9 carbon atom and the signal at 112.56 ppm was assigned to C10 carbon atom.

There are remaining three signals in which the signal at 121.20 ppm was assigned for aromatic C1 (*para*) carbon atom.

Remaining other two signals were assigned for (Cβ) C5 and (Cα) C6 carbon atoms. The down field signal at 144.00 ppm was assigned for C5 carbon atom and the upfield signal at 130.62 ppm was assigned at 130.62 ppm was assigned for C6 carbon atom, this is due to the π-bond polarization α, β unsaturated carbonyl compound.

In *para* substituted derivatives assignments of the benzene ring (C3,3’, C2.2’, C4, C1) carbon signals and C6, C8 carbon signals somewhat ambiguous in nature, which has been removed by empirical additivity rules (Appendix-I) and relative intensity. The 13C NMR chemical shift data for *para*-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones (Fig. ) are listed in table ().

**Table ( ): 13C NMR Chemical shifts of p-substituted E-(1)-(furan-2-yl)-3-phenylprop-2-ene-1-ones.**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **S.No.** | ***p*-X** | **C1** | **C2,2’** | **C3,3’** | **C4** | **C5** | **C6** | **C7** | **C8** | **C9** | **C10** | **C11** |
| 1 | **-**NMe2 | 154.26 | 111.82 | 130.53 | 122.54 | 144.86 | 116.38 | 178.29 | 152.10 | 115.94 | 112.28 | 145.86 |
| 2 | **-**CH3 |  |  |  |  |  |  |  |  |  |  |  |
| 3 | **-**H | 121.20 | 128.54 | 128.96 | 134.75 | 144.00 | 130.62 | 178.03 | 153.73 | 117.52 | 112.56 | 146.53 |
| 4 | -Cl | 153.64 | 129.67 | 129.25 | 133.26 | 142.48 | 121.63 | 177.76 | 136.52 | 117.65 | 112.65 | 146.61 |
| 5 | **-**F | 153.70 | 116.24 | 116.02 | 120.93 | 142.66 | 130.44 | 177.85 | 130.40 | 117.49 | 112.60 | 146.52 |
| 6 | **-**CHO |  |  |  |  |  |  |  |  |  |  |  |

**Substituent effects on the cyclic voltammetric reduction peak potentials of substituted (Z)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones.**

(E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one is an aromatic ketone that forms the central core for a variety of important biological compounds. Chemically they consist of open chain flavonoids in which the ends of a three carbon α, β-unsaturated carbonyl system is attached to a 2-furyl group and a substituted phenyl group. Some of the chalcone derivatives show antibacterial, antifungal, antitumor and anti-inflammatory properties1(DV2).Chalcone derivatives possess conjugated double bonds and a completely delocalized π-electron system on both rings. Molecules possessing such system have relatively low redox potentials and have a greater probability of undergoing electron transfer reactions(6)(DV1).

Electrochemical methods have proved to be very sensitive for the determination of organic molecules, including drugs and related molecules in pharmaceutical dosage forms and biological fluids(4-8)DV2.A review of the literature reveals that many studies for the electrochemical behavior of chalconeDV1,DV2 at a glassy carbon electrode are available. Hence 4’-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one are chosen in the present investigation.

It was felt that the nature of reduction at glassy carbon electrode and the effect of substituents on the reduction could be investigated with this compound.

The applicability of the LFER to cyclic voltammetry is being examined in the present investigation. Therefore, measurements of the electrochemical parameters of *para*-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one have been made by using cyclic voltammetry technique. The cyclic voltammetry technique is used to follow the reduction of these compounds since cyclic voltammetry technique possesses merits over polarography.226 The cyclic voltammetry technique has been used to characterize the reduction process.

The applicability of Hammett equation to the polarographic reduction potentials of a large variety of organic compounds, such as 4-styrylpyridines, azo dyes, styryl dyes etc. have been examined. 227,234-239 Good LFER relationships were obtained with the E1/2 values and various substituent parameters. In this part, the effect of substituents in cathodic reactions of 4’-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one is reported. In this study acetonitrile containing tetrabutylammonium tetrafluoroborate (TBATFB) as a supporting electrolyte has been used as the medium. Throughout the study, oxygen is completely removed from the cell by purging and blanketing nitrogen gas for a minimum of half an hour. After checking the deoxygenation by running a background cyclic voltammogram, the substrate is added and cyclic voltammograms were recorded. The cyclic voltammograms of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one in acetonitrile at various concentrations and at various sweep rates were recorded. The sweep rate has been changed from 20 mV s-1 to 160 mV s-1. Typical cyclic voltammograms at various sweep rates and at constant concentration (10 mm) of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one in acetonitrile is shown in figure 1.

In all the above cases, two well-defined voltammetric peaks are observed in the potential region -1.309 to -1.348 V and -1.543 to -1.563 V. There is a small anodic peak is observed in the reverse scan for the first peak. This indicates the quasi-reversibility of the reaction under the experimental conditions employed. The first peak current (ip) is proportional to the square root of sweep rate (ν1/2) at a constant concentration (10 mm) (fig.2) which is expected for a simple diffusion controlled process.216 Dr.KR

In addition, there is a linear relationship between log ip and log ν, corresponding to the following equations (1) and (2) for the first peak and second peak respectively figures (3) and (4).

log ip = 0.515 log ν + 2.850 (1)

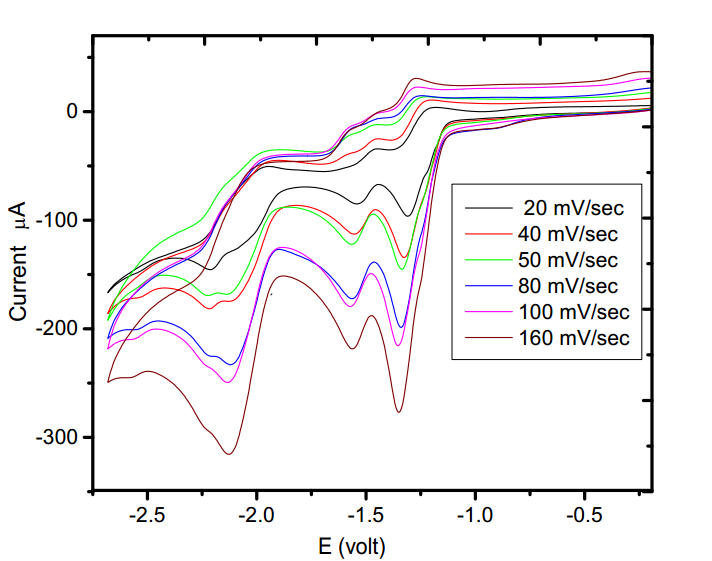
r = 0.998

and

log ip = 0.474 log ν + 2.725 (2)

r = 0.993

The slopes of 0.515 and 0.474 are close to the theoretically expected value of 0.5 for a diffusion controlled process19 DV2.

 Fig. (1). Cyclic voltammograms of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one

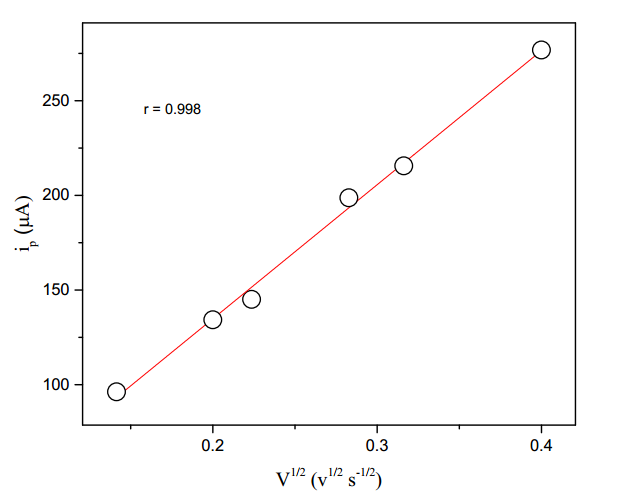
(10 mM) in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; Working electrode = glossy carbon;

Sweep rate = 20 mV/s, 40 mV/s, 50 mV/s, 80 mV/s, 100 mV/s and

160 mV/s.

.



ν1/2 (ν1/2 s1/2)

Fig.2. Plot of first peak current (ip) versus square root of sweep rates for the electrolytic

reduction of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one (10 mM) in tetrabutyl

ammonium tetrafluoroborate.

Solvent = acetonitrile.

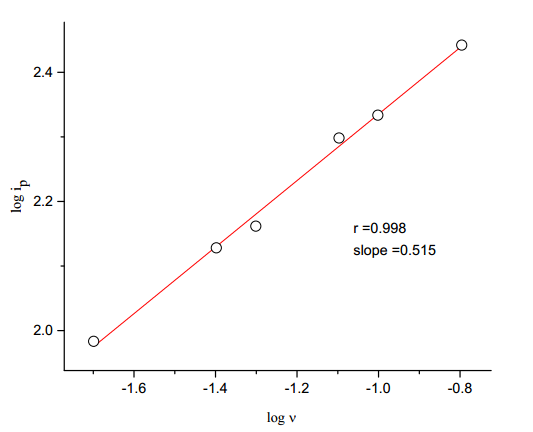


Fig. (3). Plot of logarithm of peak current on logarithm of scan rate for the first peak

for the electrolytic reduction of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one

(10 mM) in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile.

.

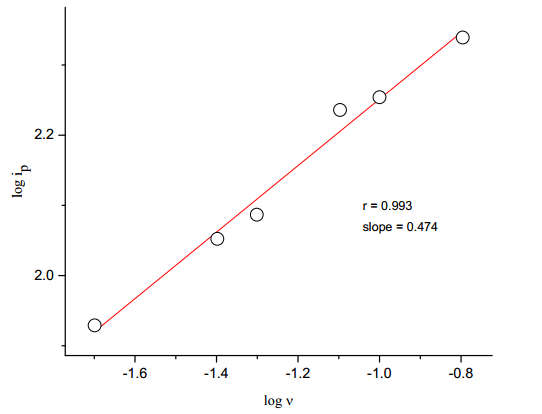


Fig. (4). Plot of logarithm of peak current on logarithm of sweep rate for the second peak

for the electrolytic reduction of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one

(10 mM) in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile.

.

The cyclic voltammograms of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one in acetonitrile containing tetrabutylammonium tetrafluoro borate at various concentration and at constant sweep rate (40 mV s-1) are shown in fig. (5). The first peak current is proportional to the concentration of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one at constant sweep rate (40 mV s-1) fig. (6).

The peak potential shifts cathodically and the shifts are very small with an increase in sweep rate and concentration, and there is a small anodic peak for the first peak which is characteristic of quasi-reversible charge transfer reaction. There is a linear dependence of Ep of the first peak vs log ν (Fig.7) (correlation coefficient, r= 0.927) also confirms that the system corresponds to the quasi-reversible cyclic voltammetric pattern. The peak current function ip/ACν1/2 where A is the area of the electrode, C is the substrate concentration and ν is the sweep rate, remains almost constant (Table 1). The above facts suggest that the electrochemical reduction is quasi-reversible and involves diffusion controlled electron transfer. Similar observations are also observed for the second peak (see Figs. 8 &9).

The differences between peak potentials and half-peak potentials (Ep - Ep1/2 ) are also nearly constant. The transfer coefficient (αna) calculated by using equation (3) is found to be a fraction (Table 1). As an example, the αna value is found to be 0.43 for the parent compound at 40

mV s-1 sweep rate and 10 mM concentration.

Ep - Ep1/2 = (-0.048)/αna (3)

The diffusion coefficient (D) of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one is taken as 3.11487 x 10-4 Cm2 s-1 for the related compound from the literature.DV1 Using these values and according to the quasi-reversible electrode process, Ip is defined by the equation20 DV2 (4)

Ip = 2.69 × 105 × n (αna)1/2 × A × D1/2 × ν1/2 × C (4)

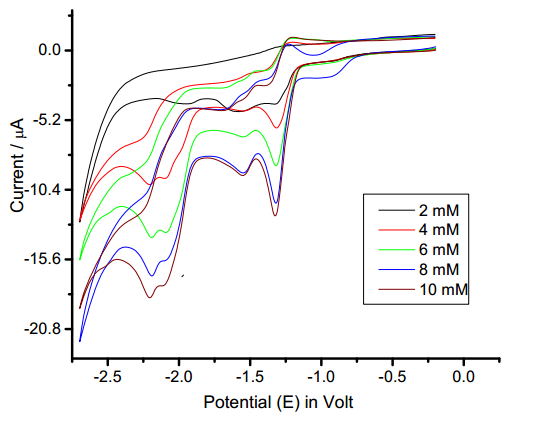


Fig. 5. Cyclic voltammograms of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one

in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; Sweep rate = 40 mV/s ; working electrode = glassy carbon

[substrate] =2 mM; 4 mM; 6 mM; 8 mM and 10 mM

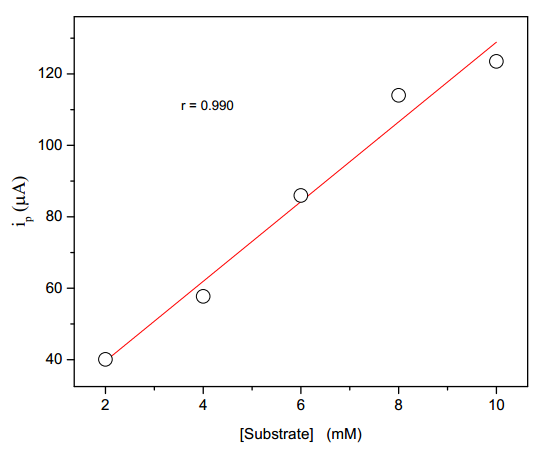
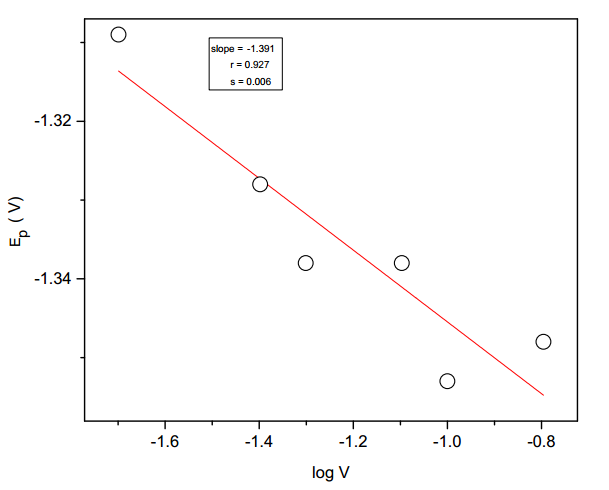


Fig.6. Plot of first peak current (ip) versus concentration of (E)-1-(furan-2-yl)-3-

phenylprop-2-ene-1-one in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; Sweep rate = 40 mV/s

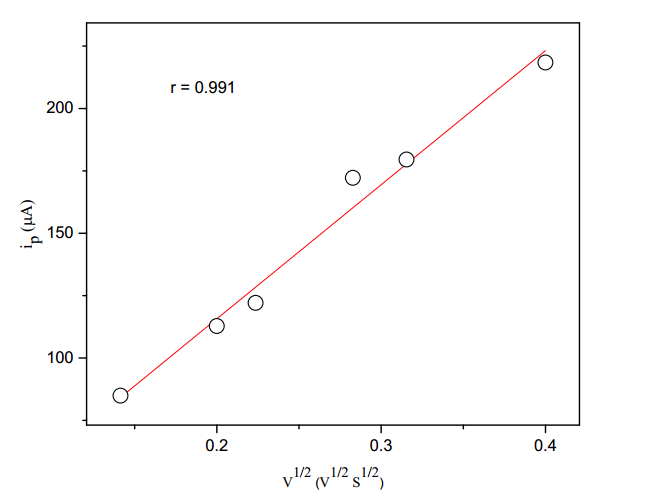


log ν

Fig.7. Plot of Ep of first peak versus log ν for the electrolytic reduction of (E)-1-

(furan-2-yl)-3-phenylprop-2-ene-1-one in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile.



ν1/2 (ν1/2s1/2)

Fig.8. Plot of second peak current (ip) versus square root of sweep rate for the

electrolytic reduction of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one in tetrabutyl

ammonium tetrafluoroborate.

Solvent = acetonitrile.

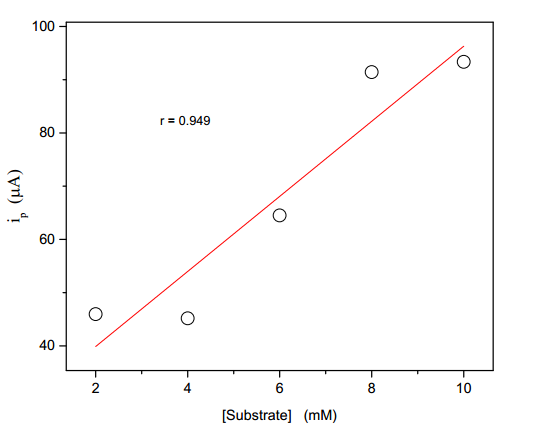


Fig. 9. Plot of second peak (ip) versus concentration of (E)-1-(furan-2-yl)-3-

phenylprop-2-ene-1-one in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; sweep rate = 40 mV/s.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | | Table (1): Cyclic voltammetric data of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one reduction on  glassy carbon electrode in acetonitrile at sweep rate 40 mV s-1. | | | | | | | | | | | | | | | | |
|  |  |  | | |  | | |  |  |  |  |  | |  | | |  |  |  | |
|  |  | First peak | | | | | | | |  | Second peak | | | | | | | | |
| S.No | [Substrate] | ip | | ip/ACν1/2 | -Ep | - Ep1/2 | αna | | |  | ip | ip/ACν1/2 | -Ep | | - Ep1/2 | αna | | | |
|  | (mM) | (µA) | |  | (V) | (V) |  | | |  | (µA) |  | (V) | | (V) |  | | | |
|  |  |  | |  |  |  |  | | |  |  |  |  | |  |  | | | |
| 1 | 2 | 40.07 | | 3190 | 1.318 | 1.216 | 0.47 | | |  | 45.97 | 3660 | 1.530 | | 1.235 | 0.16 | | | |
|  | 4 | 57.71 | | 2297 | 1.315 | 1.232 | 0.58 | | |  | 45.17 | 1798 | 1.529 | | 1.232 | 0.16 | | | |
|  | 6 | 85.97 | | 2281 | 1.320 | 1.232 | 0.55 | | |  | 64.51 | 1712 | 1.550 | | 1.114 | 0.11 | | | |
|  | 8 | 114.00 | | 2269 | 1.325 | 1.249 | 0.63 | | |  | 91.43 | 1819 | 1.550 | | 1.349 | 0.24 | | | |
|  | 10 | 123.50 | | 1967 | 1.328 | 1.241 | 0.55 | | |  | 93.35 | 1491 | 1.554 | | 1.290 | 0.18 | | | |
|  |  |  | |  |  |  |  | | |  |  |  |  | |  |  | | | |

where α is the transfer coefficient, na the number of electrons transferred, ν the scan rate, A is the electrode area, D is the diffusion coefficient and C is the concentration of electroactive spices. Thus, for the first peak the value of αna is calculated from equation (3) as 0.466 V, ip from graph as 198.7 µA, area of the electrode A is 0.0314 cm2, the scan rate ν is 80 mV and the concentration C is 10 mM for which the number electrons transferred ‘n’ for the first stage of reduction using equation (4) was calculated to be 0.979 ≈ 1.

Similarly, for the second peak the value of αna is calculated from equation (3) as 0.253 V, ip from graph as 172.2 µA, area of the electrode A is 0.0314 cm2, the scan rate ν is 80 mV and the concentration C is 10 mM for which the number electrons transferred ‘n’ for the second stage of reduction using equation (4) was calculated to be 0.81 ≈ 1. Thus, an overall number of electrons transferred is calculated to be 2.

The present investigation reveals that (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one and 4’-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones in acetonitrile take place in two successive stages at well-separated cathode potentials to give two-electron reduction process. From the observed facts and already available literature for similar compounds such as styrylpyridine231 and 4-(chlorostyryl) pyridine235 where the carbon-carbon double bond was reduced electrochemically, the electrochemical reduction mechanism of (E)-1-(Furan-2-yl)-3-phenylprop-2-ene-1-one shown in scheme 1 may be proposed.

The course of reduction of (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one (a) is probably the addition of one electron to the lowest-energy antibonding molecular orbital to give the anion radical (b) which may undergo protonation at the most basic centre, the oxygen atom. This gives a radical of which, (c) is one canonical form. The radical appears to be reduced further to a carbanion which may be protonated to give (d).



Scheme 1.

**Substituent effect**

The cyclic voltammograms for various 4’- substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones were also measured at constant [substrate] and at varying sweep rate. The cyclic voltammograms of 4’- substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones are shown in Figs. 10,11 and 12. By employing similar procedure adopted for parent compound the calculation of αna was made for all the substituent compounds. The αna values are found to have fractional values. The voltammetry responses of 4’- substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones are collected in Table 2. Analysis of these values of peak potentials reveals that the peak potentials increases cathodically with an increase in sweep rate for all the 4’- substituted

(E)-1-(Furan-2-yl)-3-phenylprop-2-ene-1-ones.

The parameters αna and current function, irreversible and diffusion controlled nature of reduction lie practically in the same range for all the members of the series. Therefore, it is possible to apply the Hammett relation to the series.103DrKR For this purpose the peak potentials and half-peak potentials for (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-one derivatives with substituents in the phenyl ring were considered for the correlation. The results of statistical analysis are described in Table 3 and the results are given by equations (5 - 24).

Correlation analysis with Ep values for the first peak

Ep = 0.350 *σ*p  - 1.285 (5)

r = 0.993; s = 0.019; ψ = 0.145

[substrate] = 10 mM; sweep rate = 20 mV s-1

Ep = 0.353 *σ*p  - 1.294 (6)

r = 0.991; s = 0.022; ψ = 0.164

[substrate] = 10 mM; sweep rate = 40 mV s-1

Ep = 0.349 *σ*p  - 1.311 (7)

r = 0.974; s = 0.039; ψ = 0.277

[substrate] = 10 mM; sweep rate = 80 mV s-1

Ep = 0.348 *σ*p  - 1.325 (8)

r = 0.992; s = 0.022; ψ = 0.155

[substrate] = 10 mM; sweep rate = 160 mV s-1

Ep = 0.342 *σ*p  - 1.342 (9)

r = 0.989; s = 0.027; ψ = 0.191

[substrate] = 10 mM; sweep rate = 320 mV s-1

Correlation analysis with Ep1/2 values for the first peak

Ep1/2 = 0.385 *σ*p  - 1.199 (10)

r = 0.999; s = 0.008; ψ = 0.055

[substrate] = 10 mM; sweep rate = 20 mV s-1

Ep1/2 = 0.377 *σ*p  - 1.206 (11)

r = 0.998; s = 0.012; ψ = 0.077

[substrate] = 10 mM; sweep rate = 40 mV s-1

Ep1/2 = 0.371 *σ*p  - 1.204 (12)

r = 0.995; s = 0.017; ψ = 0.122

[substrate] = 10 mM; sweep rate = 80 mV s-1

Ep1/2 = 0.362 *σ*p  - 1.218 (13)

r = 0.996; s = 0.014; ψ = 0.109

[substrate] = 10 mM; sweep rate = 160 mV s-1

Ep1/2 = 0.339 *σ*p  - 1.221 (14)

r = 0.989; s = 0.027; ψ = 0.191

[substrate] = 10 mM; sweep rate = 160 mV s-1

Correlation analysis with Ep values for the second peak

Ep = 0.311 *σ*p / *σ*p-  - 1.731 (15)

r = 0.857; s = 0.126; ψ = 0.631

[substrate] = 10 mM; sweep rate = 20 mV s-1

Ep = 0.307 *σ*p / *σ*p-  - 1.736 (16)

r = 0.855; s = 0.126; ψ = 0.635

[substrate] = 10 mM; sweep rate = 40 mV s-1

Ep = 0.297 *σ*p / *σ*p-  - 1.749 (17)

r = 0.839; s = 0.130; ψ = 0.666

[substrate] = 10 mM; sweep rate = 80 mV s-1

Ep = 0.293 *σ*p / *σ*p-  - 1.756 (18)

r = 0.826; s = 0.135; ψ = 0.690

[substrate] = 10 mM; sweep rate = 160 mV s-1

Ep = 0.301 *σ*p / *σ*p-  - 1.870 (19)

r = 0.920; s = 0.099; ψ = 0.506

[substrate] = 10 mM; sweep rate = 320 mV s-1

Correlation analysis with Ep1/2 values for the second peak

Ep1/2 = 0.298 *σ*p / *σ*p-  - 1.580 (20)

r = 0.833; s = 0.134; ψ = 0.678

[substrate] = 10 mM; sweep rate = 20 mV s-1

Ep1/2 = 0.285 *σ*p / *σ*p-  - 1.580 (21)

r = 0.813; s = 0.138; ψ = 0.713

[substrate] = 10 mM; sweep rate = 40 mV s-1

Ep1/2 = 0.285 *σ*p / *σ*p-  - 1.578 (22)

r = 0.839; s = 0.130; ψ = 0.666

[substrate] = 10 mM; sweep rate = 80 mV s-1

Ep1/2 = 0.288 *σ*p / *σ*p-  - 1.560 (23)

r = 0.826; s = 0.135; ψ = 0.690

[substrate] = 10 mM; sweep rate = 160 mV s-1

Ep1/2 = 0.286 *σ*p / *σ*p-  - 1.620 (24)

r = 0.838; s = 0.099; ψ = 0.506

[substrate] = 10 mM; sweep rate = 320 mV s-1

The corresponding Hammett plots Ep vs σp at 40 mV s-1, Ep1/2 vs σp at 40 mV s-1 for the first peak and Ep vs σp /σp- at 320 mV s-1, Ep1/2 vs σp/σp- at 320 mV s-1 for the second peak are illustrated in Figs.13,14,15 and 16. The Hammett correlation of Ep vs σp at 40 mV s-1 for the first peak shows an excellent correlation ( r=0.993 ). The Hammett correlation for the second peak is poor. This result is in agreement with the results for 4-(4-halostyryl)pyridines235DrKR. This is





Fig.10. Cyclic voltammograms for (a) (E)-1-(furan-2-yl)-3-(4’-N, N-dimethylaminophenyl)-

prop-2-ene-1-ones and (b) (E)-1-(furan-2-yl)-3-(4’-methylaminophenyl)-prop-2-ene-1-

one in tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; working electrode = glassy carbon; Sweep rate = 40 mv/s



(b)

(a)

(a)

Fig.11. Cyclic voltammograms for (a) (E)-1-(furan-2-yl)-3-(4’-chlorophenyl)-prop-

2-ene-1-one and (b) (E)-1-(furan-2-yl)-3-(4’-flurophenyl)-prop-2-ene-1-one in tetra

butylammonium tetrafluoroborate.

Solvent = acetonitrile; working electrode = glassy carbon; Sweep rate = 40 mv/s



Fig. 12. Cyclic voltammogram for (E)-1-(furan-2-yl)-3-(4’-oxophenyl)-prop-2-ene-1-one in

tetrabutylammonium tetrafluoroborate.

Solvent = acetonitrile; working electrode = glassy carbon; Sweep rate = 40 mv/s

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Table (2): Cyclic voltammetric data of *para*-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-ene-1-ones reduction on  glassy carbon electrode in acetonitrile  [substrate] = 10 mM | | | | | | | | | | | | |
|  | | |  |  |  |  |  |  |  |  |  |  |
|  | | | First peak  --------------------------------------------------------- | | | | | Second peak  -------------------------------------------------------------- | | | | |
|
| S.No. | Substituent | Sweep | ip | ip/ACν1/2 | -Ep | - Ep1/2 | αna | ip | ip/ACν1/2 | -Ep | - Ep1/2 | αna |
|  |  | rate |  |  |  |  |  |  |  |  |  |  |
|  |  | (mV s-1) | (µA) |  | (V) | (V) |  | (µA) |  | (V) | (V) |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 1 | NMe2 | 20 | 81.67 | 1839 | 1.567 | 1.512 | 0.87 | 65.86 | 1483 | 1.964 | 1.809 | 0.31 |
|  |  | 40 | 116.60 | 1857 | 1.577 | 1.510 | 0.72 | 91.43 | 1456 | 1.966 | 1.788 | 0.27 |
|  |  | 80 | 158.20 | 1781 | 1.590 | 1.508 | 0.59 | 125.30 | 1411 | 1.966 | 1.789 | 0.27 |
|  |  | 160 | 215.90 | 1719 | 1.608 | 1.510 | 0.49 | 178.60 | 1422 | 1.974 | 1.784 | 0.25 |
|  |  | 320 | 295.50 | 1664 | 1.621 | 1.492 | 0.37 | 262.40 | 1477 | 1.984 | 1.765 | 0.22 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 2 | Me | 20 | 66.16 | 1490 | 1.350 | 1.274 | 0.63 | 65.95 | 1485 | 1.824 | 1.667 | 0.31 |
|  |  | 40 | 87.60 | 1395 | 1.355 | 1.277 | 0.62 | 76.42 | 1217 | 1.819 | 1.657 | 0.30 |
|  |  | 80 | 139.80 | 1579 | 1.365 | 1.261 | 0.46 | 111.10 | 1251 | 1.819 | 1.650 | 0.28 |
|  |  | 160 | 201.20 | 1602 | 1.378 | 1.281 | 0.49 | 177.60 | 1414 | 1.827 | 1.626 | 0.24 |
|  |  | 320 | 267.90 | 1508 | 1.396 | 1.282 | 0.42 | 238.30 | 1342 | 1.840 | 1.639 | 0.23 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 3 | H | 20 | 96.25 | 2167 | 1.309 | 1.206 | 0.47 | 84.93 | 1913 | 1.543 | 1.384 | 0.30 |
|  |  | 40 | 134.30 | 2139 | 1.328 | 1.216 | 0.43 | 112.80 | 1796 | 1.553 | 1.384 | 0.28 |
|  |  | 50 | 145.10 | 2067 | 1.338 | 1.226 | 0.43 | 122.10 | 1739 | 1.568 | 1.389 | 0.27 |
|  |  | 80 | 198.70 | 2237 | 1.338 | 1.231 | 0.45 | 172.20 | 1939 | 1.568 | 1.378 | 0.25 |
|  |  | 100 | 215.60 | 2171 | 1.353 | 1.233 | 0.40 | 174.50 | 1757 | 1.573 | 1.390 | 0.26 |
|  |  | 160 | 276.80 | 2204 | 1.348 | 1.236 | 0.43 | 218.40 | 1739 | 1.563 | 1.329 | 0.21 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 4 | F | 20 | 19.71 | 444 | 1.270 | 1.169 | 0.48 | 87.18 | 1963 | 1.838 | 1.729 | 0.44 |
|  |  | 40 | 27.20 | 433 | 1.270 | 1.191 | 0.61 | 104.80 | 1669 | 1.848 | 1.730 | 0.41 |
|  |  | 80 | 38.83 | 437 | 1.277 | 1.168 | 0.44 | 128.27 | 1444 | 1.875 | 1.736 | 0.35 |
|  |  | 160 | 42.77 | 341 | 1.321 | 1.206 | 0.42 | 179.33 | 1428 | 1.884 | 1.766 | 0.41 |
|  |  | 320 | 64.14 | 361 | 1.357 | 1.237 | 0.40 | 232.66 | 1310 | 1.90 | 1.807 | 0.52 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 5 | Cl | 20 | 99.18 | 2233 | 1.176 | 1.112 | 0.75 | 88.60 | 1995 | 1.748 | 1.552 | 0.24 |
|  |  | 40 | 148.50 | 2365 | 1.184 | 1.114 | 0.69 | 117.50 | 1871 | 1.756 | 1.585 | 0.28 |
|  |  | 80 | 201.60 | 2270 | 1.197 | 1.116 | 0.60 | 149.60 | 1684 | 1.776 | 1.581 | 0.25 |
|  |  | 160 | 290.6 | 2314 | 1.215 | 1.128 | 0.55 | 178.80 | 1796 | 1.788 | 1.534 | 0.19 |
|  |  | 320 | 392.3 | 2209 | 1.236 | 1.13 | 0.45 | 305.80 | 1722 | 1.802 | 1.578 | 0.21 |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| 6 | CHO | 20 | 70.01 | 1577 | 1.137 | 1.028 | 0.44 | 66.44 | 1496 | 1.368 | 1.243 | 0.38 |
|  |  | 40 | 100.70 | 1604 | 1.147 | 1.034 | 0.42 | 91.03 | 1450 | 1.375 | 1.240 | 0.36 |
|  |  | 80 | 145.70 | 1641 | 1.160 | 1.040 | 0.40 | 129.30 | 1456 | 1.391 | 1.239 | 0.32 |
|  |  | 160 | 210.30 | 1674 | 1.178 | 1.051 | 0.38 | 187.40 | 1492 | 1.404 | 1.230 | 0.28 |
|  |  | 320 | 296.30 | 1668 | 1.196 | 1.060 | 0.35 | 267.60 | 1507 | 1.412 | 1.226 | 0.26 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | | Table (3). Hammett correlations for the voltammetric reduction of *para*-substituted (E)-1-(furan-2-yl)-3-phenylprop-2-  ene-1-ones on glassy carbon electrode in acetonitrile | | | | | | | | | | | | |
|  |  | |
|  |  | | [substrate] = 10 mM supporting electrolyte = tetrabutylammonium tetrafluoroborate | | | | | | | | | | | | |
|  | | | | first peak | | | | | |  |  | Second peak | | | |
|  |
| Quantity | | Substituent | | Sweep | correlation | slope | standard | n | ψ |  | correlation | slope | standard | n | ψ |
| correlated | | constant | | rate | coefficient |  | deviation |  |  |  | coefficient |  | deviation |  |  |
|  | |  | | (mV/s) |  |  |  |  |  |  |  |  |  |  |  |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
| Ep(V) | | σp | | 20 | 0.993 | 0.350±0.020 | 0.019 | 6 | 0.145 |  | 0.747 | 0.378±0.168 | 0.163 | 6 | 0.814 |
|  | |  | | 40 | 0.991 | 0.353±0.023 | 0.022 | 6 | 0.164 |  | 0.743 | 0.371±0.167 | 0.162 | 6 | 0.820 |
|  | |  | | 80 | 0.974 | 0.349±0.040 | 0.039 | 6 | 0.277 |  | 0.718 | 0.353±0.171 | 0.166 | 6 | 0.852 |
|  | |  | | 160 | 0.992 | 0.348±0.022 | 0.022 | 6 | 0.155 |  | 0.709 | 0.350±0.174 | 0.169 | 6 | 0.864 |
|  | |  | | 320 | 0.989 | 0.342±0.028 | 0.027 | 5 | 0.191 |  | 0.745 | 0.340±0.176 | 0.170 | 5 | 0.861 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp / σp- | | 20 | 0.931 | 0.236±0.046 | 0.062 | 6 | 0.447 |  | 0.857 | 0.311±0.094 | 0.126 | 6 | 0.631 |
|  | |  | | 40 | 0.927 | 0.237±0.048 | 0.064 | 6 | 0.459 |  | 0.855 | 0.307±0.093 | 0.126 | 6 | 0.635 |
|  | |  | | 80 | 0.919 | 0.237±0.050 | 0.068 | 6 | 0.483 |  | 0.839 | 0.297±0.096 | 0.130 | 6 | 0.666 |
|  | |  | | 160 | 0.930 | 0.234±0.046 | 0.062 | 6 | 0.450 |  | 0.826 | 0.293±0.100 | 0.135 | 6 | 0.690 |
|  | |  | | 320 | 0.935 | 0.232±0.051 | 0.068 | 5 | 0.458 |  | 0.920 | 0.302±0.074 | 0.099 | 5 | 0.506 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp+/ σp- | | 20 | 0.958 | 0.165±0.024 | 0.049 | 6 | 0.351 |  | 0.845 | 0.209±0.066 | 0.131 | 6 | 0.655 |
|  | |  | | 40 | 0.953 | 0.166±0.026 | 0.052 | 6 | 0.371 |  | 0.844 | 0.207±0.065 | 0.129 | 6 | 0.657 |
|  | |  | | 80 | 0.932 | 0.163±0.032 | 0.063 | 6 | 0.444 |  | 0.826 | 0.199±0.067 | 0.134 | 6 | 0.690 |
|  | |  | | 160 | 0.959 | 0.165±0.024 | 0.047 | 6 | 0.347 |  | 0.818 | 0.198±0.069 | 0.137 | 6 | 0.704 |
|  | |  | | 320 | 0.965 | 0.163±0.023 | 0.050 | 5 | 0.339 |  | 0.853 | 0.191±0.067 | 0.133 | 5 | 0.674 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp+/σp/ σp- | | 20 | 0.967 | 0.165±0.021 | 0.043 | 6 | 0.312 |  | 0.800 | 0.196±0.073 | 0.146 | 6 | 0.735 |
|  | |  | | 40 | 0.965 | 0.167±0.022 | 0.045 | 6 | 0.321 |  | 0.799 | 0.193±0.073 | 0.146 | 6 | 0.736 |
|  | |  | | 80 | 0.949 | 0.165±0.027 | 0.055 | 6 | 0.386 |  | 0.780 | 0.186±0.075 | 0.149 | 6 | 0.766 |
|  | |  | | 160 | 0.970 | 0.165±0.021 | 0.042 | 6 | 0.298 |  | 0.771 | 0.185±0.076 | 0.153 | 6 | 0.780 |
|  | |  | | 320 | 0.970 | 0.162±0.023 | 0.046 | 5 | 0.314 |  | 0.815 | 0.180±0.074 | 0.147 | 5 | 0.748 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
| Ep1/2 (V) | | σp | | 20 | 0.999 | 0.385±0.008 | 0.008 | 6 | 0.055 |  | 0.741 | 0.369±0.167 | 0.162 | 6 | 0.822 |
|  | |  | | 40 | 0.998 | 0.376±0.012 | 0.012 | 6 | 0.077 |  | 0.700 | 0.342±0.174 | 0.168 | 6 | 0.875 |
|  | |  | | 80 | 0.995 | 0.371±0.017 | 0.017 | 6 | 0.122 |  | 0.697 | 0.343±0.176 | 0.171 | 6 | 0.878 |
|  | |  | | 160 | 0.996 | 0.362±0.015 | 0.014 | 6 | 0.109 |  | 0.673 | 0.353±0.194 | 0.188 | 6 | 0.906 |
|  | |  | | 320 | 0.989 | 0.339±0.028 | 0.027 | 5 | 0.191 |  | 0.651 | 0.309±0.208 | 0.201 | 5 | 0.980 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp / σp- | | 20 | 0.947 | 0.262±0.044 | 0.060 | 6 | 0.393 |  | 0.833 | 0.298±0.099 | 0.134 | 6 | 0.678 |
|  | |  | | 40 | 0.952 | 0.258±0.041 | 0.056 | 6 | 0.375 |  | 0.813 | 0.285±0.102 | 0.138 | 6 | 0.713 |
|  | |  | | 80 | 0.942 | 0.252±0.044 | 0.060 | 6 | 0.411 |  | 0.839 | 0.297±0.096 | 0.130 | 6 | 0.666 |
|  | |  | | 160 | 0.953 | 0.249±0.039 | 0.053 | 6 | 0.371 |  | 0.826 | 0.294±0.100 | 0.135 | 6 | 0.690 |
|  | |  | | 320 | 0.957 | 0.235±0.041 | 0.055 | 5 | 0.375 |  | 0.838 | 0.286±0.107 | 0.099 | 5 | 0.506 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp+/ σp- | | 20 | 0.977 | 0.184±0.019 | 0.039 | 6 | 0.261 |  | 0.846 | 0.209±0.066 | 0.131 | 6 | 0.653 |
|  | |  | | 40 | 0.978 | 0.181±0.019 | 0.037 | 6 | 0.255 |  | 0.803 | 0.192±0.071 | 0.141 | 6 | 0.730 |
|  | |  | | 80 | 0.970 | 0.177±0.022 | 0.044 | 6 | 0.298 |  | 0.800 | 0.193±0.072 | 0.143 | 6 | 0.735 |
|  | |  | | 160 | 0.977 | 0.174±0.018 | 0.037 | 6 | 0.261 |  | 0.768 | 0.197±0.082 | 0.162 | 6 | 0.784 |
|  | |  | | 320 | 0.977 | 0.164±0.021 | 0.040 | 5 | 0.275 |  | 0.762 | 0.178±0.087 | 0.172 | 5 | 0.836 |
|  | |  | |  |  |  |  |  |  |  |  |  |  |  |  |
|  | | σp+/σp/ σp- | | 20 | 0.983 | 0.183±0.016 | 0.033 | 6 | 0.225 |  | 0.783 | 0.189±0.075 | 0.151 | 6 | 0.762 |
|  | |  | | 40 | 0.983 | 0.180±0.016 | 0.033 | 6 | 0.225 |  | 0.755 | 0.179±0.077 | 0.155 | 6 | 0.803 |
|  | |  | | 80 | 0.982 | 0.177±0.017 | 0.034 | 6 | 0.231 |  | 0.752 | 0.179±0.078 | 0.157 | 6 | 0.807 |
|  | |  | | 160 | 0.983 | 0.173±0.016 | 0.032 | 6 | 0.225 |  | 0.720 | 0.183±0.088 | 0.176 | 6 | 0.850 |
|  | |  | | 320 | 0.978 | 0.162±0.020 | 0.040 | 5 | 0.269 |  | 0.720 | 0.166±0.090 | 0.184 | 5 | 0.896 |

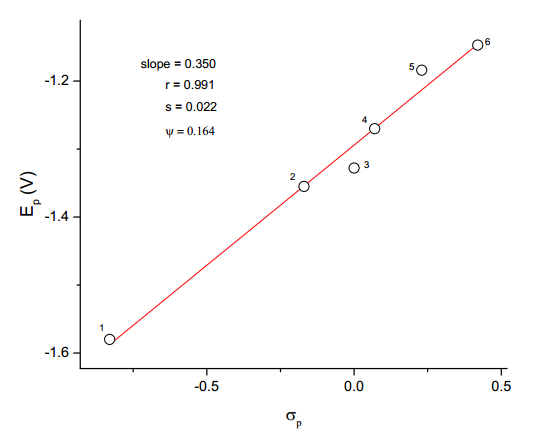


Fig. 13. Hammett plot for the electrolytic reduction of substituted (E)-1-(furan-2-yl)-

3-(4’-phenyl)-prop-2-ene-1-ones.

(first peak; numbering as in Table 2.). Sweep rate = 40 mV/s.

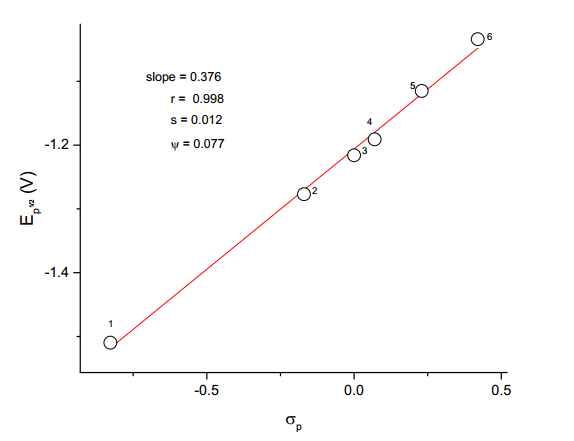


Fig.14. Hammett plot for the electrolytic reduction of substituted (E)-1-(furan-2-yl)-

3-(4’-phenyl)-prop-2-ene-1-ones.

(first peak; numbering as in Table 2.). Sweep rate = 40 mV/s.

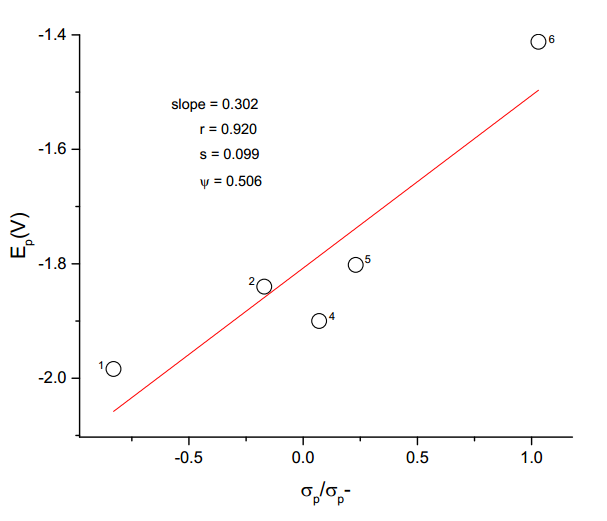


Fig. 15. Hammett plot for the electrolytic reduction of substituted (E)-1-(furan-2-yl)-

3-(4’-phenyl)-prop-2-ene-1-ones.

(second peak; numbering as in Table 2). Sweep rate = 320 mV/s.

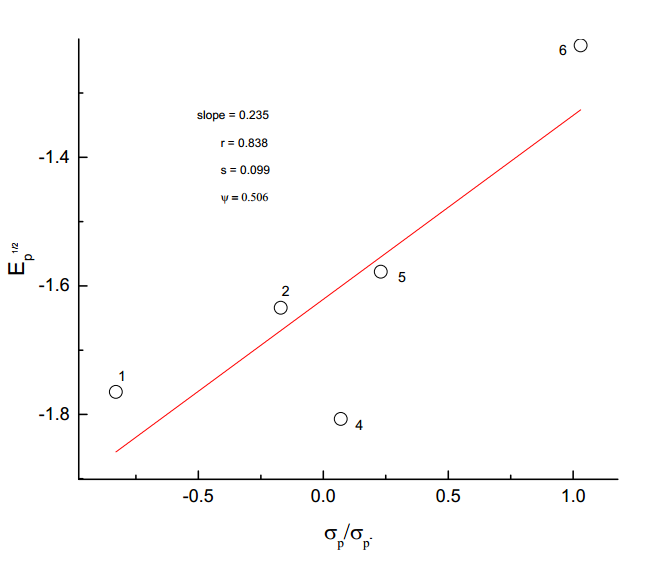


Fig. 16. Hammett plot for the electrolytic reduction of substituted (E)-1-(furan-2-yl)-

3-(4’-phenyl)-prop-2-ene-1-ones.

(second peak; numbering as in Table 2 ). Sweep rate = 320 mV/s.