Supporting Information

The Syntheses, Spectro-electrochemical Studies, Molecular and Electronic Structures of Ferrocenyl Ene-diynes

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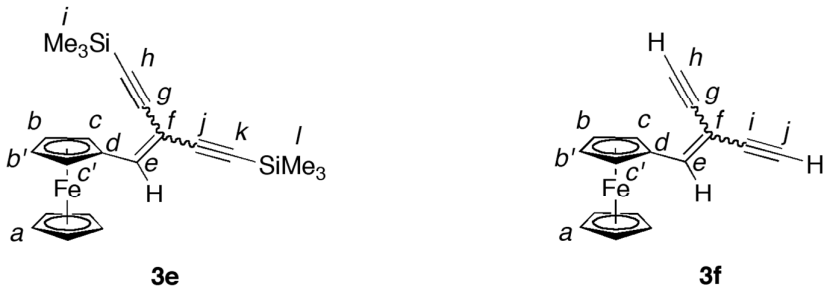

Figure S-1 The NMR labelling scheme for **3e** and **3f**.

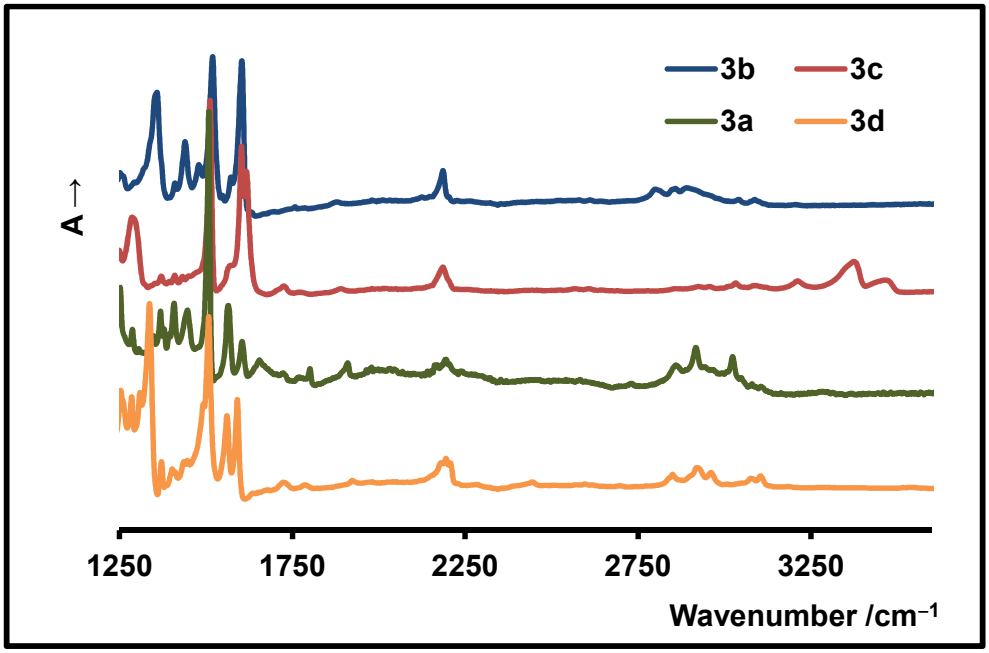

Figure S2. ATR-FTIR spectra obtained from solid **3a-d**.

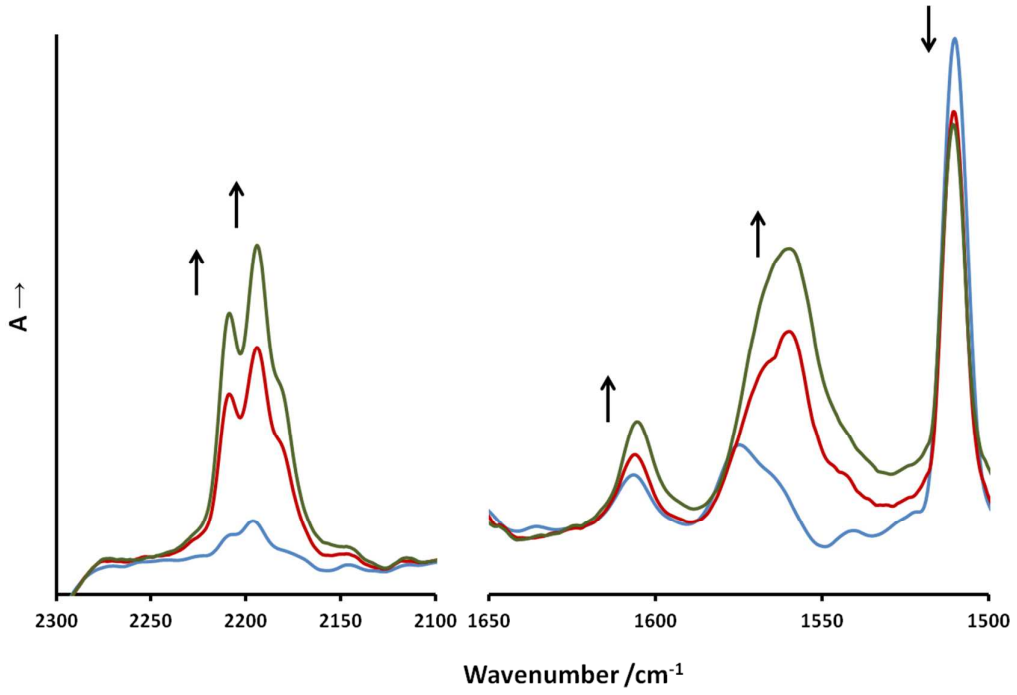

Figure S3. Reversible IR spectral changes resulting from the ferrocenyl-centered electrochemical oxidation of **3a** in CH_2Cl_2 / 10^{-1} M Bu_4NPF_6 within an OTTLE cell.

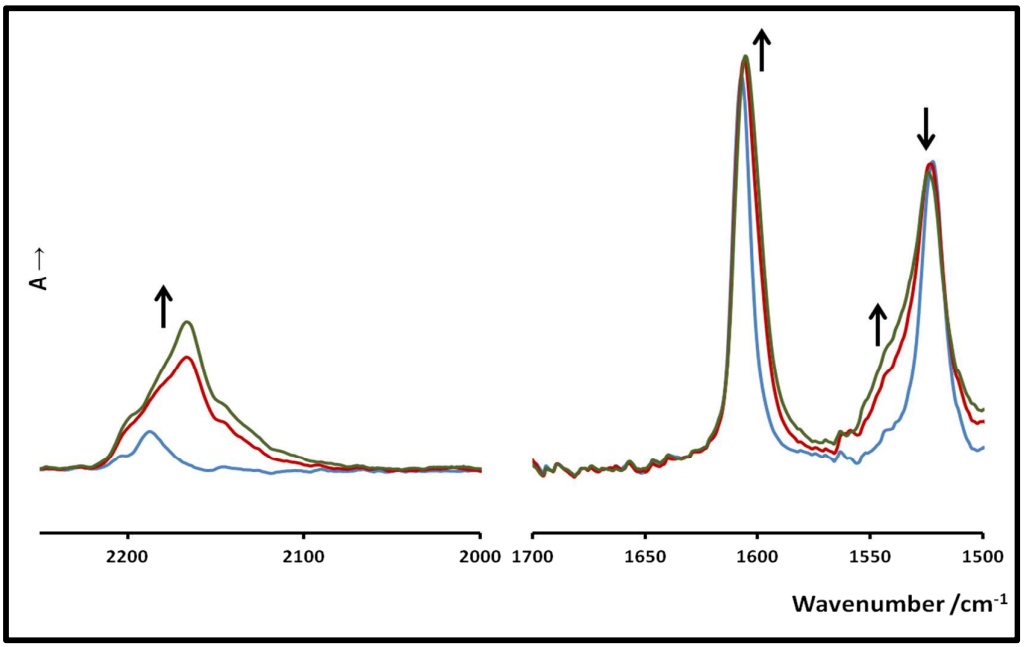

Figure S4. IR spectral changes resulting from the ferrocenyl-centered electrochemical oxidation of **3b** in CH_2Cl_2 / 10^{-1} M Bu_4NPF_6 within an OTTLE cell.

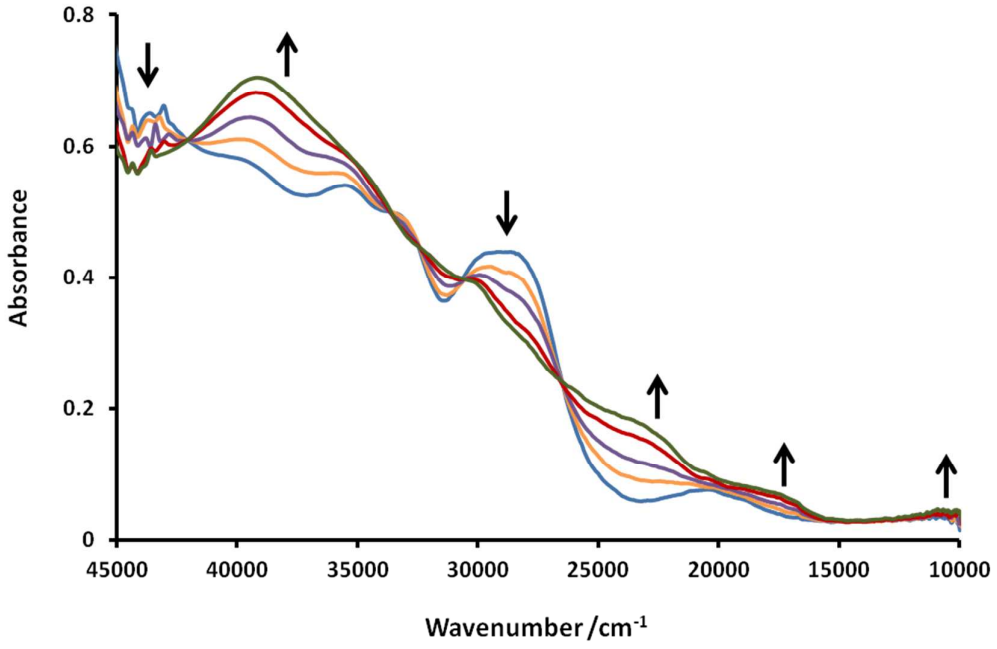

Figure S5. Reversible UV-Vis-NIR spectral changes resulting from the ferrocenyl-centered electrochemical oxidation of **3a** in CH_2Cl_2 / 10^{-1} M Bu_4NPF_6 within an OTTLE cell.

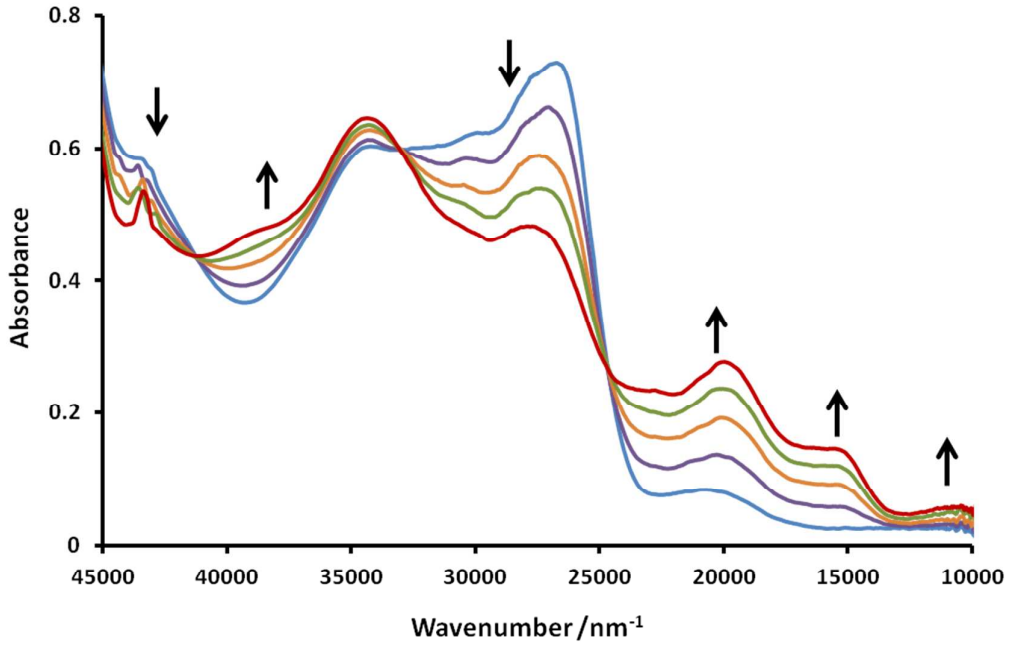

Figure S6. Reversible UV-Vis-NIR spectral changes resulting from the ferrocenyl-centered electrochemical oxidation of **3b** in CH_2Cl_2 / 10^{-1} M Bu_4NPF_6 within an OTTLE cell.

Table S1. Cartesian coordinates for **3a´** and [**3a´**]$^+$.

	3a´			[**3a´**]$^+$		
C	8.129677	10.249522	6.413052	8.163029	10.052975	6.364206
C	7.142878	10.072237	5.404575	7.159731	9.862042	5.371378
C	7.546443	8.983588	4.580846	7.587889	8.819448	4.507545
C	8.781991	8.487368	5.083138	8.859048	8.373717	4.951694
C	9.143787	9.270306	6.213833	9.216888	9.130866	6.101639
Fe	8.992041	10.489865	4.525006	8.995999	10.462348	4.479213
C	9.148223	12.467960	3.888836	9.090589	12.540898	3.961783
C	10.401686	12.046248	4.452978	10.378579	12.165635	4.464523
C	10.851596	10.925767	3.676131	10.838704	11.083875	3.640092
C	9.903539	10.688138	2.649375	9.874485	10.849863	2.622261
C	8.853222	11.640901	2.778714	8.790855	11.752061	2.824757
C	10.988674	12.683799	5.614537	10.972707	12.784684	5.628077
C	12.236350	12.540787	6.150607	12.222343	12.596933	6.152567
C	13.257294	11.688546	5.621044	13.213493	11.718730	5.620305
C	14.169074	10.998639	5.212085	14.115483	11.010762	5.218461
C	15.236892	10.183612	4.722398	15.180008	10.184662	4.748147
C	15.168786	9.593195	3.446036	15.118166	9.574926	3.480392
C	16.210590	8.804325	2.977454	16.162775	8.779327	3.032848

C	17.356131	8.571956	3.753177	17.301763	8.559657	3.823066
C	17.419284	9.161885	5.021041	17.357120	9.168771	5.082914
C	16.382311	9.954270	5.503233	16.318432	9.969530	5.544026
C	18.476726	7.714743	3.228426	18.425475	7.695379	3.320178
C	12.597163	13.290568	7.318407	12.609505	13.331287	7.315543
C	12.921832	13.919280	8.305184	12.946740	13.952435	8.303122
C	13.301007	14.662357	9.466384	13.336652	14.688537	9.461817
C	12.401982	15.549614	10.081668	12.449151	15.593359	10.069186
C	12.780205	16.269154	11.210891	12.837055	16.309236	11.196082
C	14.057453	16.134135	11.766936	14.111212	16.151401	11.754923
C	14.951066	15.246653	11.149167	14.992139	15.245375	11.144430
C	14.587170	14.522696	10.022041	14.619373	14.524710	10.019253
C	14.470069	16.912343	12.987766	14.535402	16.928140	12.971426
H	10.337073	13.397269	6.117957	10.340796	13.511600	6.133888
H	8.539594	13.286840	4.259930	8.453268	13.307038	4.392812
H	7.969022	11.704950	2.153064	7.887371	11.814990	2.227003
H	9.956994	9.895116	1.910200	9.950331	10.104727	1.836764
H	11.748815	10.348457	3.857075	11.766064	10.540794	3.768090
H	8.124443	11.013829	7.184000	8.132459	10.777693	7.171749
H	6.252212	10.677853	5.270152	6.236455	10.425424	5.279853
H	7.016332	8.611894	3.709590	7.058800	8.461075	3.629780

H	9.361752	7.673381	4.659289	9.466188	7.608565	4.477907
H	10.047607	9.158960	6.804324	10.136799	9.030208	6.668906
H	14.293159	9.762507	2.822615	14.248713	9.735786	2.846300
H	16.135599	8.358965	1.985642	16.097165	8.318800	2.047684
H	18.297469	8.999309	5.644796	18.230403	9.014712	5.715056
H	16.454602	10.401793	6.492417	16.382868	10.434037	6.525682
H	15.297933	13.840094	9.560297	15.318253	13.827800	9.561122
H	15.952435	15.121208	11.560825	15.989098	15.104031	11.560788
H	12.065203	16.951173	11.669990	12.134629	17.006199	11.651419
H	11.402640	15.672474	9.668773	11.453989	15.732546	9.651729
H	19.296088	7.638248	3.951771	19.235181	7.621140	4.054116
H	18.124825	6.698250	3.004324	18.070795	6.679644	3.098038
H	18.884070	8.125560	2.294402	18.844324	8.099248	2.388339
H	13.654558	17.545578	13.354576	13.723097	17.558383	13.349574
H	14.771434	16.239527	13.802431	14.850544	16.253764	13.779161
H	15.331555	17.559449	12.771678	15.392179	17.577367	12.743472

Table S2. Cartesian coordinates for **3b´** and [**3b´**]$^+$.

	3b´			[**3b´**]$^+$		
C	8.202011	10.176727	6.484516	8.314265	10.188859	6.312306
C	7.151606	10.047604	5.528640	7.255064	10.046028	5.376986
C	7.519763	9.021843	4.582545	7.567002	8.963408	4.486042
C	8.803724	8.510098	5.006162	8.800007	8.399385	4.959388
C	9.222803	9.228793	6.161660	9.272736	9.166552	6.053627
Fe	7.424577	8.251188	6.526268	7.442933	8.314383	6.600769
C	7.407335	7.424916	8.432029	7.394537	7.597214	8.649729
C	6.137251	8.013479	8.138979	6.176812	8.244068	8.311126
C	5.604781	7.362951	6.982873	5.589798	7.538395	7.220877
C	6.544704	6.369394	6.563388	6.457787	6.461614	6.881482
C	7.658322	6.407784	7.458347	7.575158	6.507254	7.760412
C	6.806068	8.498390	3.434421	6.834754	8.421581	3.373997
C	5.649000	8.945807	2.838496	5.664353	8.878864	2.814214
C	4.894533	10.084045	3.265268	4.920779	10.004660	3.265707
C	4.201684	11.045232	3.570817	4.228904	10.955870	3.583396
C	5.121261	8.248510	1.702322	5.118223	8.201916	1.686166
C	4.652054	7.662369	0.736585	4.639753	7.633880	0.721455
H	7.268130	7.622546	2.970557	7.283225	7.547959	2.906826

H	9.353626	7.710177	4.510515	9.292335	7.533712	4.527098
H	10.147332	9.068182	6.715417	10.193167	8.995038	6.602202
H	8.210631	10.863141	7.330818	8.371882	10.939678	7.093960
H	6.225636	10.615303	5.518204	6.367315	10.662334	5.330325
H	6.440501	5.716511	5.697145	6.303788	5.741952	6.083562
H	8.551804	5.787027	7.396294	8.430303	5.838911	7.739311
H	8.075987	7.714073	9.242519	8.092355	7.913937	9.418756
H	5.670098	8.832649	8.684968	5.770357	9.127833	8.792658
H	4.660827	7.599186	6.492399	4.650586	7.782042	6.734497
C	3.391801	12.159995	3.934612	3.413358	12.060421	3.940668
C	4.109674	6.970568	-0.386134	4.086045	6.968796	-0.403472
C	3.792366	13.072767	4.937913	3.766062	12.934362	4.989353
C	3.000147	14.154605	5.298853	2.970723	14.010286	5.332948
C	1.745121	14.392654	4.671275	1.760216	14.280446	4.640136
C	1.345584	13.475127	3.658853	1.408477	13.397980	3.583505
C	2.146612	12.396989	3.306931	2.212503	12.325812	3.249776
H	4.750869	12.927856	5.442948	4.687754	12.764830	5.543181
H	3.361382	14.823677	6.079305	3.290819	14.651095	6.147715
N	0.955650	15.458914	5.026188	0.971449	15.340510	4.973606
H	0.396281	13.605738	3.140118	0.496004	13.555472	3.018297
H	1.804898	11.713247	2.525603	1.911993	11.670812	2.434094

C	2.960217	7.444587	-1.059874	2.886874	7.412268	-0.998154
C	2.424346	6.772576	-2.151291	2.342952	6.770081	-2.094280
C	3.012439	5.572527	-2.640772	2.973586	5.634055	-2.668496
C	4.169166	5.097767	-1.961684	4.180493	5.190034	-2.065596
C	4.695963	5.778464	-0.871453	4.714451	5.840315	-0.969455
H	2.479996	8.363198	-0.713159	2.377120	8.280693	-0.585186
H	1.536788	7.185717	-2.629274	1.417935	7.152914	-2.511923
N	2.487559	4.902048	-3.719779	2.443629	4.996848	-3.752013
H	4.663321	4.183922	-2.290225	4.704632	4.326705	-2.461479
H	5.585638	5.380808	-0.376656	5.641764	5.472218	-0.534556
C	3.105514	3.673166	-4.187543	3.107971	3.837402	-4.315749
C	1.301956	5.408600	-4.388878	1.208803	5.470127	-4.347128
C	-0.322283	15.673426	4.369285	-0.258187	15.594672	4.247482
C	1.392756	16.379525	6.061897	1.357494	16.228582	6.053523
H	0.631302	17.157046	6.199127	0.601084	17.008661	6.163675
H	1.538459	15.872647	7.033381	1.437650	15.696730	7.013107
H	2.343340	16.878865	5.799163	2.322884	16.718152	5.856955
H	-0.801234	16.565367	4.791763	-0.744726	16.479490	4.663985
H	-0.208380	15.833271	3.281486	-0.073003	15.781227	3.179324
H	-1.009932	14.820024	4.512181	-0.961753	14.752897	4.326445
H	1.043830	4.742690	-5.221810	0.954997	4.835828	-5.199547

H	0.430133	5.456693	-3.710742	0.369799	5.433887	-3.636401
H	1.460037	6.421545	-4.802058	1.298665	6.504662	-4.710051
H	2.546217	3.293436	-5.051168	2.534266	3.476598	-5.172168
H	4.152639	3.830044	-4.504664	4.123441	4.076057	-4.664862
H	3.106188	2.886127	-3.411009	3.186008	3.014891	-3.589272

Table S3. Cartesian coordinates for **3d′** and [**3d′**]$^+$.

	3d′			[**3d′**]$^+$		
C	8.214226	10.187632	6.420597	8.282156	10.187845	6.350211
C	7.217246	10.030531	5.437350	7.262346	10.036242	5.391829
C	7.380483	9.043100	4.445349	7.386357	9.047711	4.397318
C	8.507178	8.235700	4.433860	8.504833	8.228606	4.359066
C	9.475203	8.416561	5.419470	9.496543	8.403376	5.320415
C	9.343091	9.383143	6.414189	9.402553	9.371163	6.316878
C	6.059065	10.861935	5.443681	6.112280	10.880733	5.426512
C	5.077378	11.576293	5.450214	5.139617	11.604634	5.459005
C	3.917552	12.414479	5.437453	3.989458	12.454151	5.478091
C	2.972331	12.157783	4.396754	3.018952	12.197030	4.461820
C	2.215400	11.895565	3.484463	2.248679	11.915453	3.567227
C	1.320639	11.589535	2.416306	1.349574	11.576836	2.510690
C	0.230570	12.434873	2.130786	0.223594	12.377810	2.244507
C	-0.640774	12.135968	1.094585	-0.647481	12.045442	1.217697
C	-0.418703	10.986314	0.339809	-0.384395	10.908363	0.459058
C	0.650809	10.130917	0.595354	0.721261	10.096492	0.696205
C	1.518136	10.434730	1.633563	1.588454	10.433322	1.725171
N	-1.336103	10.668030	-0.753954	-1.303494	10.555019	-0.628222

N	10.664750	7.567444	5.408761	10.679955	7.539148	5.281612
C	3.787191	13.394388	6.383957	3.896460	13.430486	6.428775
C	2.735309	14.364428	6.576901	2.853880	14.417299	6.620455
C	1.433390	14.468213	5.976559	1.596041	14.591462	5.955410
C	0.783210	15.598740	6.526623	0.939531	15.716393	6.520039
C	1.655398	16.202775	7.477708	1.764588	16.234620	7.560254
C	2.847324	15.444733	7.521887	2.928121	15.429873	7.630896
Fe	1.242069	14.221703	8.042458	1.172611	14.267087	8.016704
C	1.069897	13.960668	10.108835	0.818829	13.875164	10.092976
C	-0.219020	14.139184	9.531476	-0.422438	14.164713	9.470122
C	-0.427677	13.092369	8.590443	-0.629104	13.214974	8.434963
C	0.732193	12.270408	8.582214	0.483678	12.326347	8.423048
C	1.657772	12.807247	9.522410	1.381050	12.737057	9.451532
H	4.611369	13.473839	7.092552	4.726516	13.501529	7.129016
H	3.709844	15.636502	8.152343	3.747064	15.549911	8.333804
H	1.432060	17.075569	8.082375	1.539936	17.086620	8.193584
H	-0.221990	15.929398	6.286112	-0.027737	16.103155	6.215795
H	1.014980	13.789145	5.245593	1.209351	13.971483	5.157596
H	2.648717	12.418197	9.734326	2.331568	12.272873	9.695510
H	1.533401	14.608345	10.846340	1.273547	14.443231	10.898642
H	-0.911672	14.944589	9.754144	-1.075988	14.997932	9.709888

H	-1.305850	12.962556	7.965822	-1.477888	13.185348	7.758720
H	0.894479	11.401819	7.952094	0.624464	11.489230	7.746669
H	0.072863	13.331558	2.724682	0.034944	13.266570	2.841292
H	-1.483384	12.780966	0.866805	-1.519320	12.654436	1.001376
H	0.792866	9.243861	-0.013462	0.892362	9.218494	0.081798
H	2.356670	9.776894	1.847298	2.457152	9.811623	1.925844
H	6.616447	8.915331	3.682652	6.601949	8.927034	3.654472
H	8.643640	7.472833	3.674215	8.615274	7.462648	3.598375
H	10.117169	9.496839	7.166456	10.196931	9.476795	7.048788
H	8.096120	10.947038	7.189454	8.190782	10.949858	7.120066
O	-1.123201	9.664875	-1.402431	-1.051048	9.568459	-1.284972
O	-2.264078	11.422521	-0.957914	-2.265973	11.268463	-0.811129
O	11.497853	7.740482	6.274019	11.533171	7.706362	6.126248
O	10.760456	6.730923	4.534825	10.742749	6.702563	4.406720

Table S4. Selected bond lengths and angles from **3d**, [**3a´**]$^{n+}$, [**3b´**]$^{n+}$ and [**3d´**]$^{n+}$ (n = 0 ,1).

	3d	**3a´**	[**3a´**]$^{+}$	**3b´**	[**3b´**]$^{+}$	**3d´**	[**3d´**]$^{+}$
C1-C11	1.445(3)	1.449	1.446	1.450	1.438	1.444	1.448
C11-C12	1.355(3)	1.365	1.368	1.376	1.376	1.369	1.366
C12-C13	1.434(3)	1.431	1.427	1.431	1.423	1.429	1.429
C13-C14	1.197(3)	1.214	1.215	1.224	1.218	1.214	1.214
C14-C15	1.435(3)	1.430	1.427	1.425	1.419	1.427	1.428
C12-C21	1.437(3)	1.434	1.429	1.433	1.424	1.431	1.430
C21-C22	1.199(3)	1.214	1.214	1.223	1.217	1.214	1.213
C22-C23	1.434(3)	1.430	1.427	1.426	1.419	1.426	1.427
C1-C11-C12	129.8(2)	129.7	128.7	129.7	128.5	130.0	128.9
C11- C12-C13	119.3(2)	124.7	125.2	124.9	125.4	124.7	125.3
C11-C12-C21	123.4(2)	119.7	119.3	119.6	119.4	119.4	119.3

Table S5. Orbital energies (E_{orb}) and contributions from Mulliken population analysis for [**3a′**]$^+$.

Orbital	E_{orb} (eV)	Contributions (%)					
		cis to ferrocene	HC=C$_{vinyl}$		FeCp$_2$	*trans* to ferrocene	
		MeC$_6$H$_4$	C≡C	HC=C$_{vinyl}$	FeCp$_2$	C≡C	C$_6$H$_4$Me
spin-density	/	0	0	0	99	0	0
117							
β*	-1.24	0	0	0	98	0	0
α*	-2.59	0	0	0	98	0	0
116							
β*	-1.98	5	6	20	56	4	4
α*	-3.20	2	4	14	68	5	2
115							
β*	-2.97	2	4	14	68	4	2
α	-6.75	10	8	24	16	15	23
114							
β	-6.70	11	9	24	12	15	23
α	-7.26	40	17	0	0	11	27
113							
β	-7.26	39	16	0	0	11	28
α	-7.99	0	0	0	0	0	99
112							
β	-7.99	0	0	0	0	0	99
α	-8.07	99	0	0	0	0	0
111							

β	-8.08	99	0	0	0	0	0
α	-8.33	19	6	11	29	4	23
110							
β	-8.39	20	9	13	21	7	24
α	-8.65	0	33	0	5	49	2
109							
β	-8.66	1	32	0	0	52	3
α	-8.76	0	0	0	93	4	0
108							
β	-8.96	0	0	0	97	0	0
α	-9.21	1	43	4	9	31	0
107							
β	-9.21	0	33	3	31	24	0
α	-9.28	4	11	9	48	14	8
106							
β	-9.23	0	18	3	54	13	0
α	-9.55	23	30	0	0	25	14
105							
β	-9.56	16	24	0	12	23	14
α	-10.20	0	0	0	96	0	0
104							
β	-9.62	0	4	0	83	5	0
α	-10.33	0	2	1	86	2	0
103							
β	-9.66	0	0	0	93	0	0
α	-10.40	0	0	0	93	0	0
96							
α	-11.30	0	0	0	90	0	1

*unoccupied orbital.

Table S6. Orbital energies (E_{orb}) and contributions from Mulliken population analysis for [**3b´**]$^+$.

Orbital	E_{orb} (eV)	Contributions (%)					
		cis to ferrocene				*trans* to ferrocene	
		$Me_2NC_6H_4$	C≡C	HC=C_{vinyl}	$FeCp_2$	C≡C	$C_6H_4NMe_2$
spin-density	/	0	0	0	101	-1	0
133							
β*	-0.99	0	0	0	98	0	0
α*	-2.36	0	0	0	98	0	0
132							
β*	-1.68	5	6	19	58	3	4
α*	-3.12	1	4	12	68	5	3
131							
β*	-2.79	3	5	14	64	5	3
α	-5.95	0	0	10	5	11	66
130							
β	-5.90	8	2	13	6	10	55
α	-6.06	72	11	4	0	1	6
129							
β	-6.07	64	10	1	0	3	17
α	-7.36	11	7	21	21	11	17
128							
β	-7.38	12	8	21	16	12	18
α	-7.95	0	0	0	0	0	99
127							

β	-7.96	0	0	0	0	0	99
α	-8.04	99	0	0	0	0	0
126							
β	-8.05	99	0	0	0	0	0
α	-8.31	29	21	0	0	18	21
125							
β	-8.34	30	21	0	0	18	22
α	-8.43	1	38	0	0	52	3
124							
β	-8.43	1	38	0	0	52	3
α	-8.61	0	0	0	96	0	0
123							
β	-8.81	0	0	0	98	0	0
α	-8.81	11	4	5	60	3	10
122							
β	-8.92	7	2	3	70	2	6
α	-9.01	3	48	3	0	36	0
121							
β	-9.01	3	47	3	0	35	0
α	-9.51	21	2	12	18	5	29
120							
β	-9.25	13	1	4	55	0	15
α	-9.95	27	17	0	7	17	21
119							
β	-9.42	0	0	0	95	0	0
α	-10.00	0	1	0	86	2	0
118							
β	-9.44	0	0	0	95	0	0

α	-10.17	0	0	0	94	0	0
117							
β	-9.45	0	0	0	95	0	0
α	-10.27	1	4	2	82	3	0
113							
α	-11.05	1	2	4	78	2	1

*unoccupied orbital.

Table S7. Orbital energies (E_{orb}) and contributions from Mulliken population analysis for [**3d´**]$^+$.

Orbital	E_{orb} (eV)	Contributions (%)					
		cis to ferrocene				*trans* to ferrocene	
		$O_2NC_6H_4$	C≡C	$HC{=}C_{vinyl}$	$FeCp_2$	C≡C	$C_6H_4NO_2$
spin-density	/	0	0	0	99	0	0
134							
β*	-1.12	4	4	11	67	1	2
131							
β*	-2.46	0	0	2	18	5	52
α*	-2.79	0	0	0	98	0	0
130							
β*	-2.54	48	5	3	28	0	0
α*	-3.48	5	5	17	53	5	4
129							
β*	-3.34	9	6	18	48	5	6
α	-7.26	8	10	27	21	17	14
128							
β	-7.23	9	11	27	17	17	15
α	-8.09	32	21	0	0	16	24
127							
β	-8.09	32	21	0	0	16	25
α	-8.56	0	0	0	0	0	98
126							
β	-8.56	0	0	0	0	0	98

α	-8.66	98	0	0	0	0	0
125							
β	-8.66	98	0	0	0	0	0
α	-8.91	0	0	1	87	0	3
124							
β	-8.99	3	30	2	7	42	6
α	-8.93	10	11	3	49	12	7
123							
β	-9.09	7	6	4	53	11	10
α	-9.03	2	26	0	12	45	4
122							
β	-9.12	3	0	0	85	4	0
α	-9.54	10	35	2	0	21	21
121							
β	-9.51	6	1	6	67	2	9
α	-9.66	13	3	0	0	9	68
120							
β	-9.54	11	35	2	0	20	20
α	-9.71	35	5	11	25	6	15
119							
β	-9.66	13	3	0	0	9	68
α	-9.75	51	14	5	8	7	7
118							
β	-9.74	67	13	0	1	6	3
α	-9.85	0	0	0	0	0	97
117							
β	-9.78	0	0	0	93	0	0
α	-9.92	97	0	0	0	0	0

116							
β	-9.86	0	0	0	0	0	97
α	-10.07	0	0	0	0	0	91
115							
β	-9.87	0	0	0	94	0	0
α	-10.13	91	0	0	0	0	0
108							
α	-11.47	0	0	1	92	0	0

*unoccupied orbital.

Table S8. Calculated excited state parameters in the range from 0 to 20000 cm^{-1}: UV-vis-NIR transition energies E_{trans}, transition dipole moments μ_{trans} and character of [**3a´**]$^+$, [**3b´**]$^+$ and [**3d´**]$^+$.[a]

	E_{trans} (cm^{-1})	μ_{trans} (D)	character
[**3a´**]$^+$	8242	0.7	interconfiguration
	11807	1.1	cross-conjugated fragment to vinyl ferrocene charge transfer
	19432	5.7	cross-conjugated fragment to vinyl ferrocene charge transfer
	19838	2.6	cross-conjugated fragment to ferrocene charge transfer
[**3b´**]$^+$	8381	1.3	interconfiguration
	10123	2.0	*trans* $Me_2NC_6H_4C{\equiv}C$ to vinyl ferrocene charge transfer
	16108	2.9	*cis* $Me_2NC_6H_4C{\equiv}C$ to vinyl ferrocene charge transfer
	16309	3.4	interconfiguration
	16560	6.2	*trans* $Me_2NC_6H_4C{\equiv}C$ to vinylferrocene charge transfer
	16678	3.8	mixed interconfiguration and charge transfer
	19640	7.2	*cis* $Me_2NC_6H_4C{\equiv}C$ to vinyl ferrocene charge transfer
[**3d´**]$^+$	8237	0.5	interconfiguration
	12168	0.7	delocalized π/π^* to vinyl ferrocene charge transfer

[a] Transitions with a $\mu_{trans} < 0.5$ D are neglected.

Table S9. Crystal data and parameters of structure refinement for **3d** and **Z-5d**

Compound	**3d**	**z-5d**
Empirical formula	$C_{28}H_{18}N_2O_4Fe$	$C_{20}H_{14}BrFeNO_2$
Formula weight	502.29	436.08
Temperature/K	120	120
Crystal system	triclinic	monoclinic
Space group	P-1	C2/c
a/Å	7.6788(6)	25.4582(13)
b/Å	9.2709(7)	11.3257(3)
c/Å	16.1965(13)	12.0048(5)
α/°	87.211(2)	90.00
β/°	81.908(2)	100.582(4)
γ/°	79.096(2)	90.00
Volume/$Å^3$	1120.64(15)	3402.5(2)
Z	2	8
ρ_{calc}mg/mm^3	1.489	1.703
m/mm^{-1}	0.713	3.248
F(000)	516.0	1744.0
Crystal size/mm^3	0.43 × 0.12 × 0.06	0.50 × 0.27 × 0.03
2Θ range for data collection	2.54 to 59°	1.5914 to 3.1592°
Index ranges	$-10 \leq h \leq 10$, $-12 \leq k \leq 12$, $-22 \leq l \leq 22$	$-34 \leq h \leq 35$, $-15 \leq k \leq 15$, $-16 \leq l \leq 16$
Reflections collected	14152	27104
Independent reflections, R_{int}	6195, 0.0341	4748, 0.0726
Data/restraints/parameters	6195/0/388	4748/0/282
Goodness-of-fit on F^2	1.047	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0406, wR_2 = 0.0905	R_1 = 0.0454, wR_2 = 0.0979
Final R indexes [all data]	R_1 = 0.0633, wR_2 = 0.1012	R_1 = 0.0684, wR_2 = 0.1076
Largest diff. peak/hole / e $Å^{-3}$	0.47/-0.38	0.78/-0.74