# Conformational-Modulated Intramolecular Electron Transfer Process in a diaza[2,2]ferrocenophane.

Francisco Otón,[a] Imma Ratera,[a] Arturo Espinosa,[b] Alberto Tarraga,[b] Jaime Veciana[a] and Pedro Molina.[b]

## Supporting Information

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[a] Prof. J. Veciana, Dra. I. Ratera, Dr. F. Otón.
*Instituto de Ciencia de los Materiales de Barcelona (CSIC)/CIBER-BBN, Campus de la Universidad Autónoma de Barcelona, Bellaterra E-08193 (Barcelona), Spain, Fax: (+34)935805729, E-mail:* ***vecianaj@icmab.es***

[b] Prof. P. Molina, Prof. A. Tárraga, Dr. A. Espinosa.
*Universidad de Murcia, Departamento de Química Orgánica, Facultad de Química, Campus de Espinardo, E-30100 Murcia, Spain, Fax: (+34) 968 364149, E-mail:* ***pmolina@um.es*** *and* ***atarraga@um.es***

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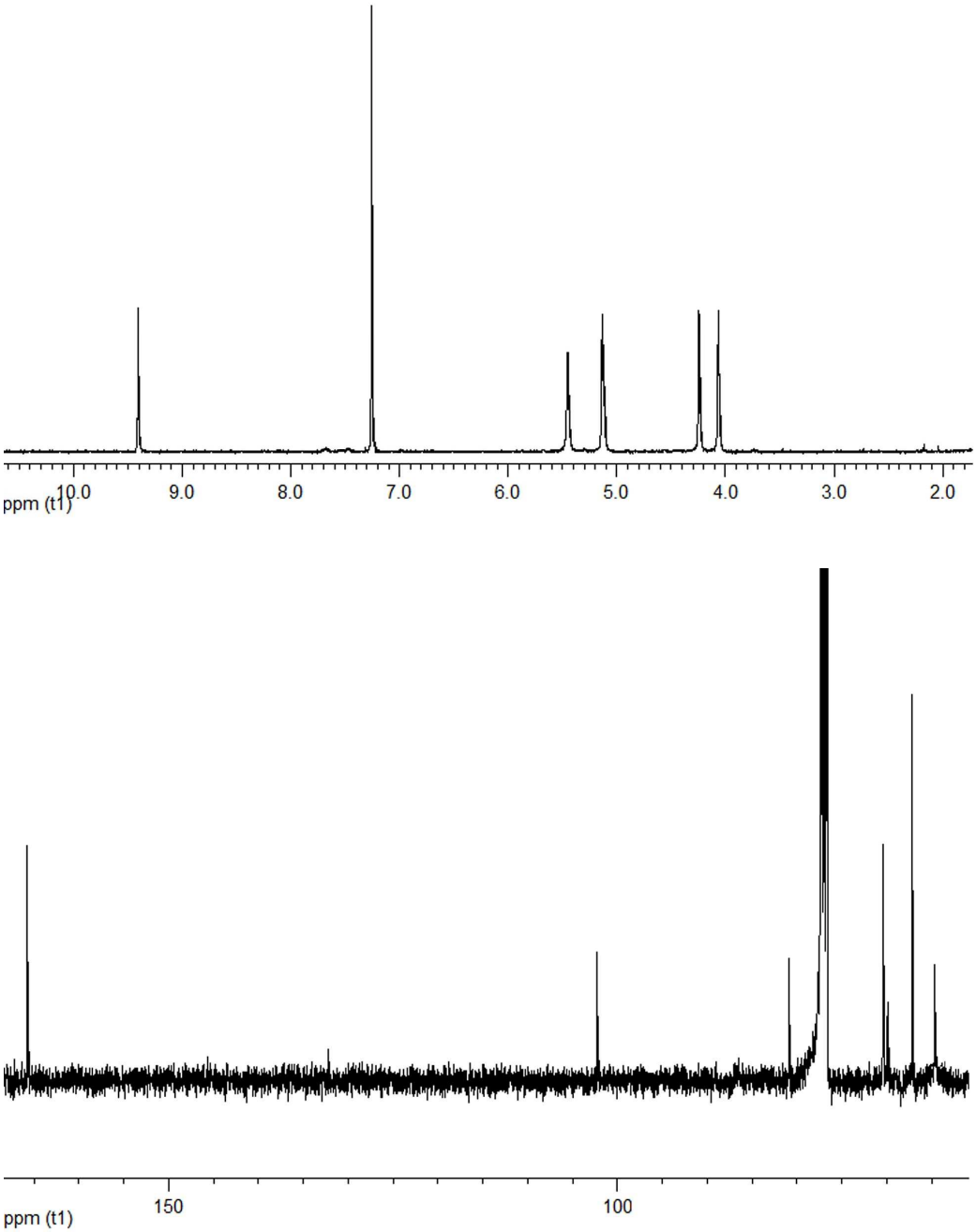


**Figure S1.** Top: $^{1}$H NMR (200 MHz, $CDCl_3$) and Bottom: $^{13}$C NMR (100.4 MHz, $CDCl_3$) of bis(methylidenamino)[2,2](1,1´´,1´,1´´´)ferrocenophane, **3.**

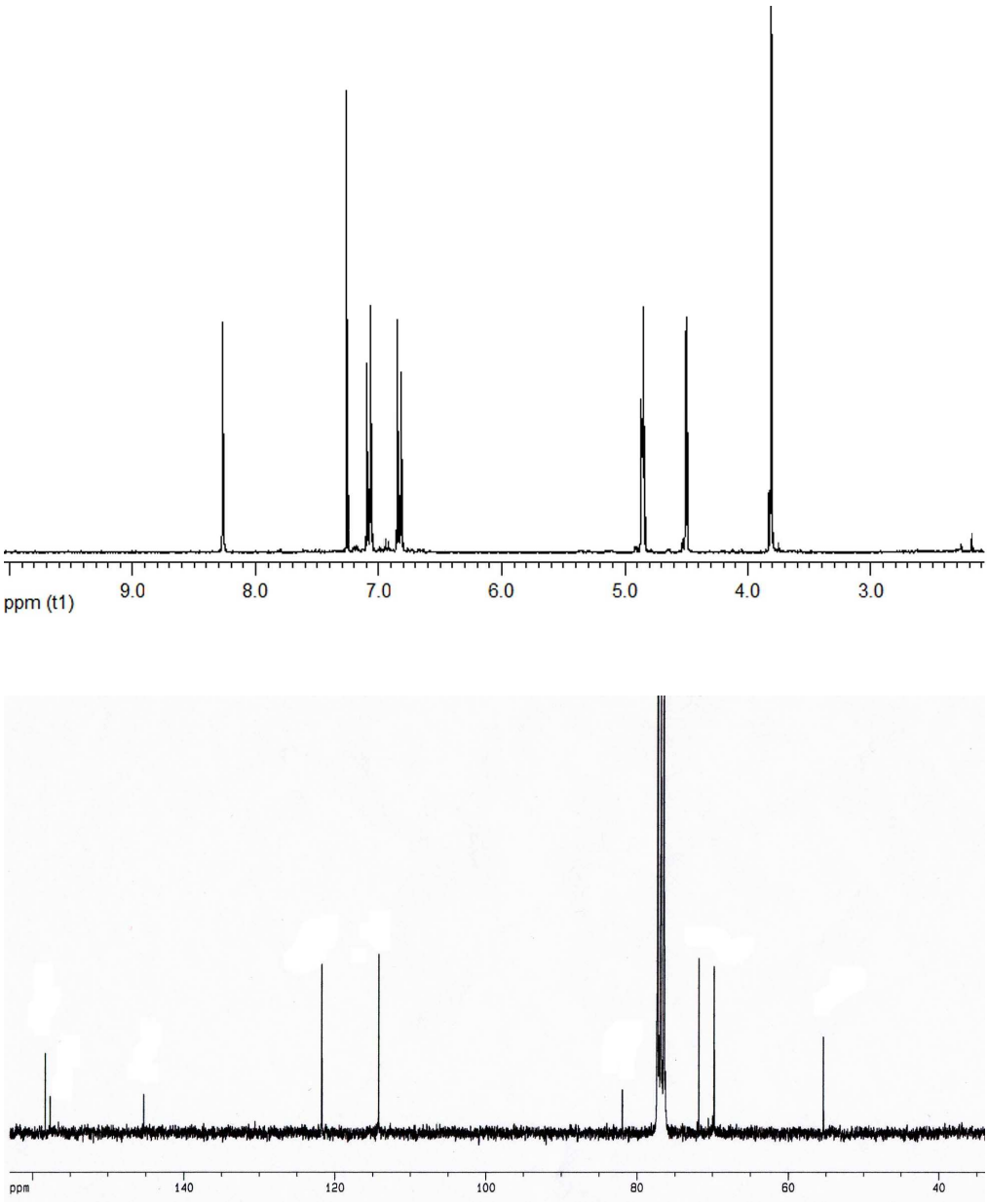


**Figure S2.** Top: $^{1}H$ NMR (300 MHz, $CDCl_3$) and Bottom: $^{13}C$ NMR (75.3 MHz, $CDCl_3$) of 1,1´-Bis[(4-metoxyphenylimino)methyl)ferrocene, **4.**

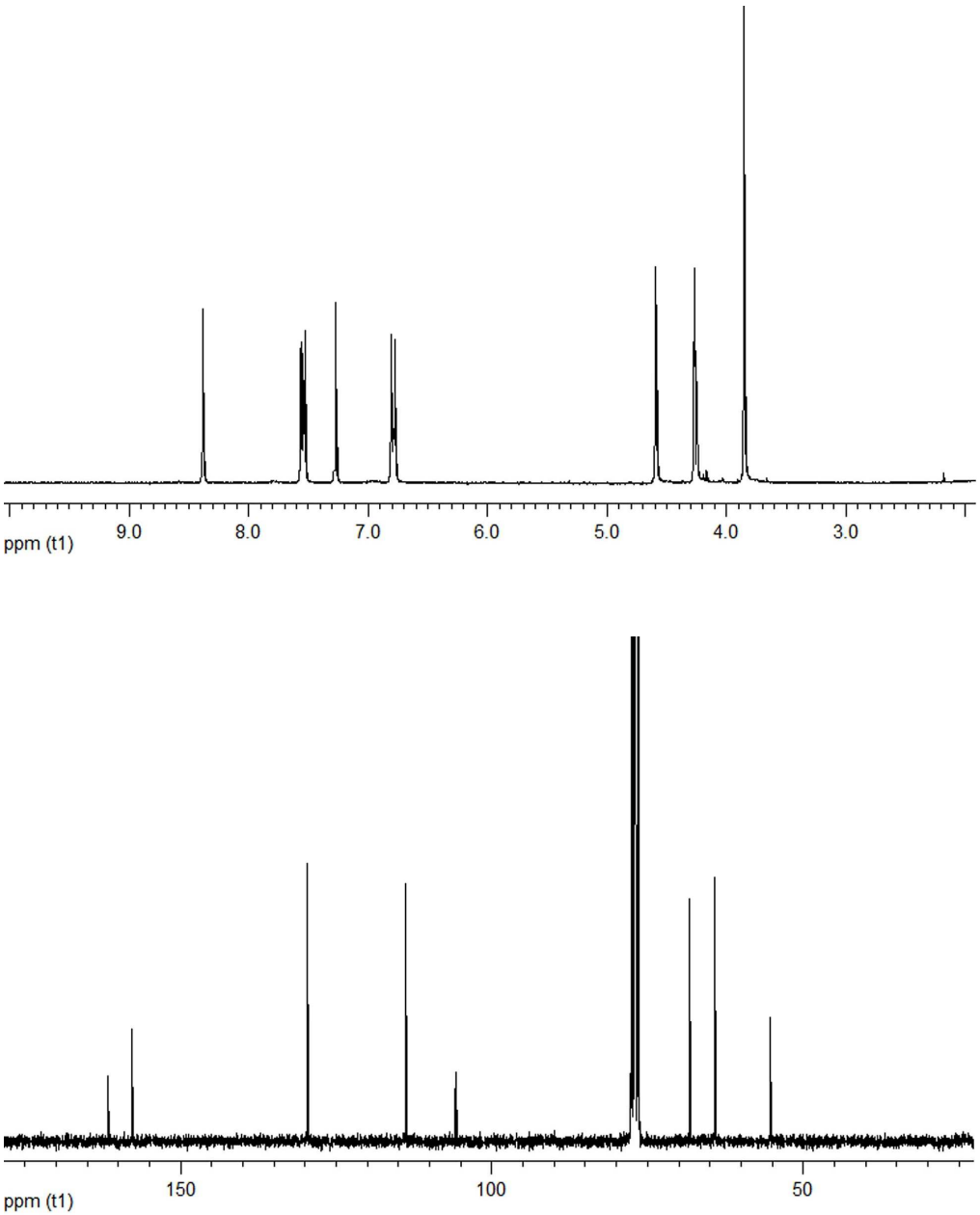


**Figure S3.** Top: $^{1}H$ NMR (300 MHz, $CDCl_3$) and Bottom: $^{13}C$ NMR (75.3 MHz, $CDCl_3$) of 1,1´-bis(4-metoxybenzylidenamino)ferrocene, **5.**

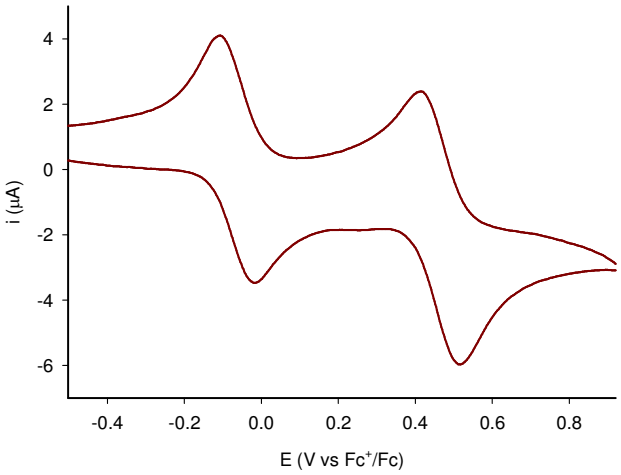


**Figure S4.** CV of **3** (1 x $10^{-3}$ M) scanned at 0.1 $Vs^{-1}$ in $CH_2Cl_2$ using $[(n\text{-}Bu)_4N]PF_6$ (0.1 M) as supporting electrolyte.

**Table S1.** Electrochemical data for compounds **3, 4** and **5** obtained from different solvents.

| Solvent | Compound | $E^1_{1/2}$ (V) | $E^2_{1/2}$ (V) | $\Delta E_{1/2}$ [a] (mV) | $E^2_{1/2}$ (3) - $E_{1/2}$ (5) [b] (mV) |
|---|---|---|---|---|---|
| $CH_2Cl_2$ | **3** | - 0.06 | 0.45 | 510 | |
| $CH_2Cl_2$ | **4** | ---- | 0.22 | | |
| | | | | | 230 |
| $CH_2Cl_2$ | **5** | - 0.07 | ---- | | |
| THF | **3** | - 0.07 | 0.42 | 490 | |
| THF | **4** | ---- | 0.21 | | |
| | | | | | 210 |
| THF | **5** | - 0.06 | ---- | | |
| DMF | **3** | - 0.01 | 0.43 | 440 | |
| DMF | **4** | ---- | 0.22 | | |
| | | | | | 210 |
| DMF | **5** | - 0.07 | ---- | | |
| EtOH | **3** | 0.02 | 0.29 | 310 | |
| EtOH | **4** | ---- | 0.24 | | |
| | | | | | 50 |
| EtOH | **5** | 0.04 | ---- | | |

[a] $\Delta E_{1/2} = E^2_{1/2} - E^1_{1/2}$; being $E^1_{1/2}$ the oxidation potential corresponding to the ferrocene moiety directly linked to the N of the imine bridge and $E^2_{1/2}$ the corresponding to the ferrocene moiety linked to the CH of such bridge; [b] $E^2_{1/2}$ **(3)** and $E_{1/2}$ **(4)** correspond to the second oxidation potential of compound **3** and to the oxidation potential of compound **4**, respectively, obtained from the indicated solvents.

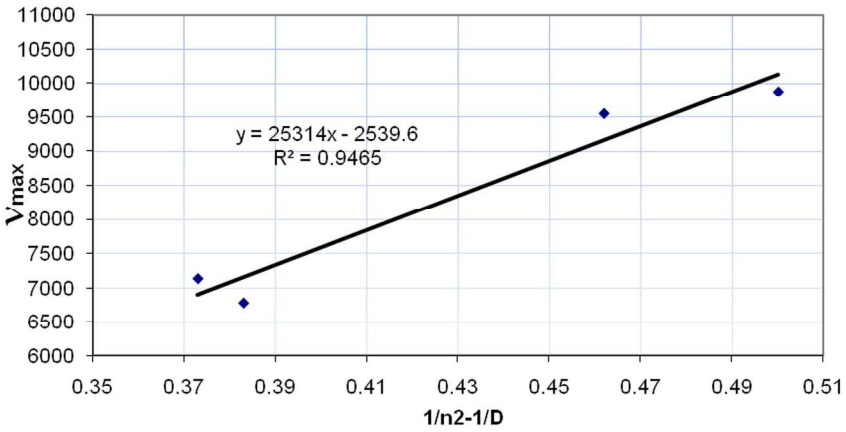


**Figure S5.** Plot of the values of $\nu_{max}$ *vs* $1/n^2$-1/D (*n* is the refractive index and *D* the dielectric constant) for different solvents and linear regression of data of compound **3**.

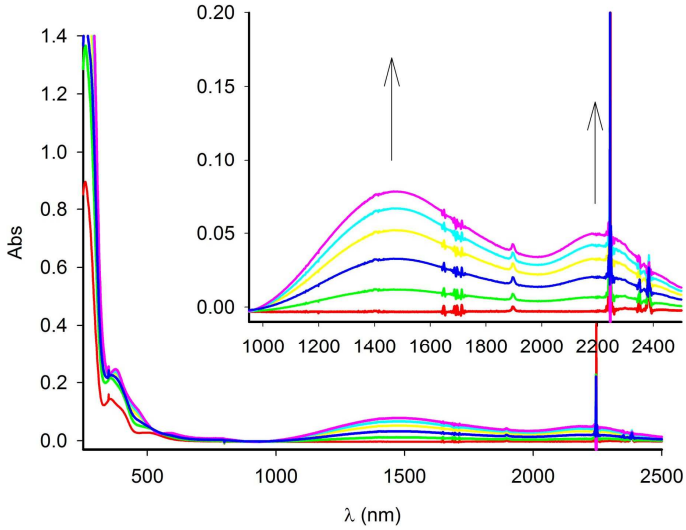


**Figure S6.** Evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **3** in $CH_2Cl_2$ with $[(n\text{-}Bu)_4N]PF_6$ (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electrons are removed. Arrows indicate absorptions that increase or decrease during the experiment.

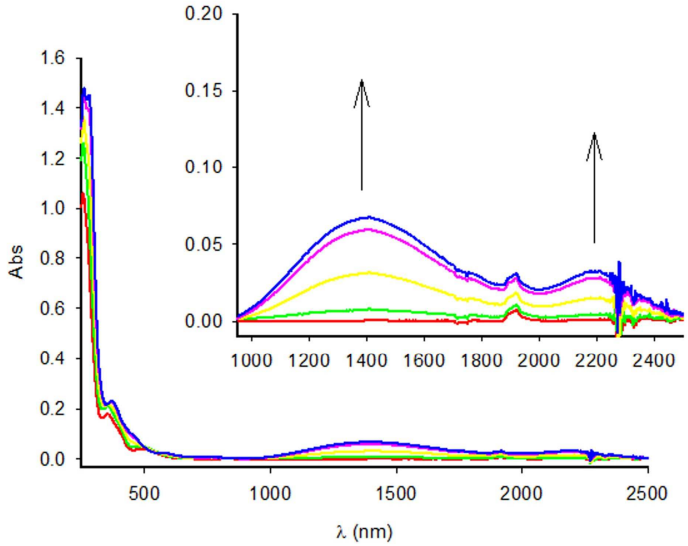


**Figure S7.** Evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **3** in THF with $[(n\text{-Bu})_4\text{N}]PF_6$ (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electrons are removed. Arrows indicate absorptions that increase or decrease during the experiment.

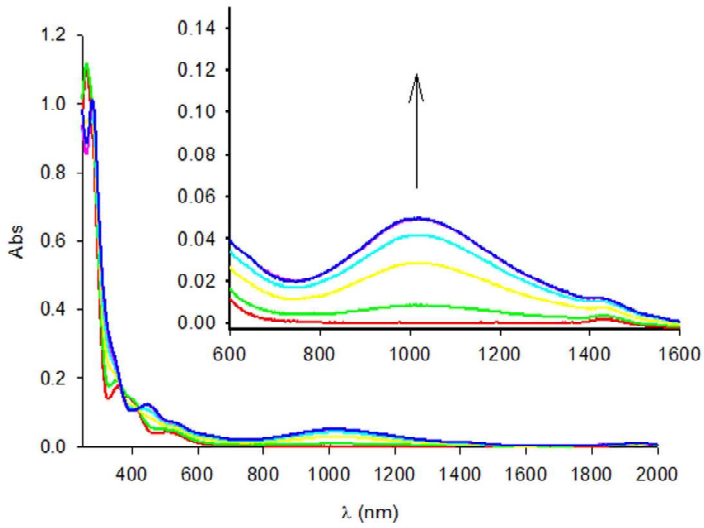


**Figure S8.** Evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **3** in EtOH with $[(n\text{-Bu})_4\text{N}]PF_6$ (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electrons are removed. Arrows indicate absorptions that increase or decrease during the experiment.

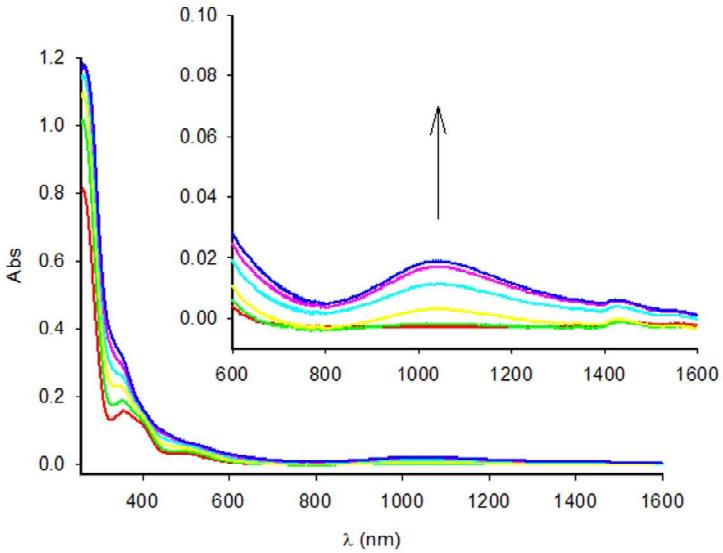


**Figure S9.** Evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **3** in DMF with $[(n\text{-Bu})_4\text{N}]PF_6$ (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electrons are removed. Arrows indicate absorptions that increase or decrease during the experiment.

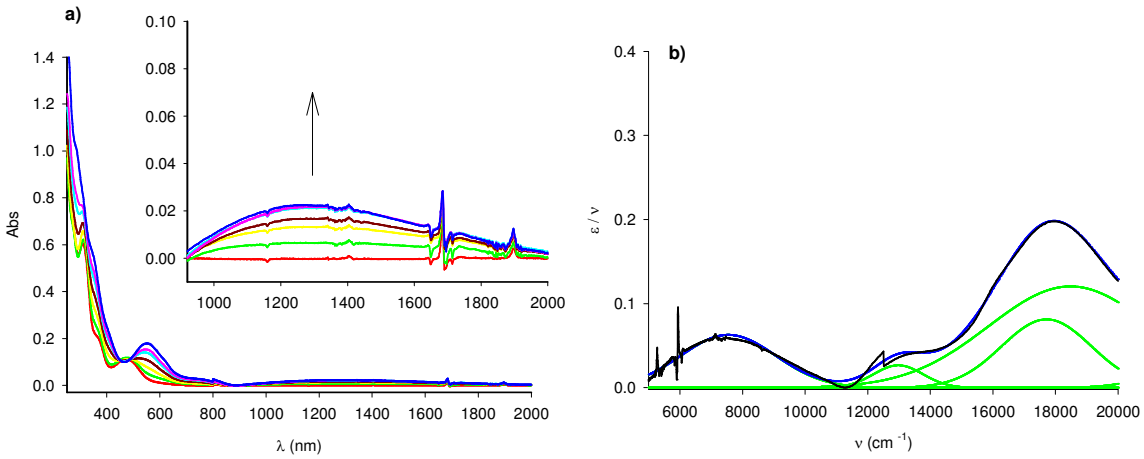


**Figure S10.** a) Evolution of UV-Vis-NIR spectra during the course of the oxidation of compound **6** in $CH_2Cl_2$ with $[(n\text{-Bu})_4\text{N}]PF_6$ (0.15 M) as supporting electrolyte when $0 \leq n \leq 1$ electrons are removed. Arrows indicate absorptions that increase or decrease during the experiment. b) Deconvolution of the espectra of the mixed valence compound $\mathbf{6}^{+\bullet}$. Experimental data (black) were deconvoluted by means of gaussian functions using spectra intensity times wavenumbers vs wavenumbers. The sum of the deconvoluted spectra (blue) closely matches the lowest energy part of the experimental spectrum.

**Details of the RI-BP86/Def2-TZVP theoretical calculations.**

At this level, the TD calculation (computed at the same COSMO/RI-BP86/Def2-TZVP level taking 20 roots, with maximum dimension 60 and including quadruplets) for the $[\mathbf{3}\boldsymbol{qC_s}]^{+\bullet}$ isomer in $CH_2Cl_2$ predicts only one significant (with high oscillator strength $f$=0.0976) band at λ=1069.2 nm mainly corresponding to a βHOMO-3→βLUMO (SOMO) (with also some βHOMO→βLUMO contribution). The second most intense band in the NIR region is expected to be ca. 25-times weaker ($f$=0.0039). That is why we assume that the only possible source for the second lower energy and less intense experimentally observed band could be the only significant band in this region calculated for the other $[\mathbf{3}\boldsymbol{C_2}]^{+\bullet}$ isomer, which is expected to be a bit less intense ($f$=0.0772) and shifted to lower energies (λ=1180.5 nm), while being originated from an slightly different electronic transition mainly of βHOMO→βLUMO type (in this case with also some βHOMO-3→βLUMO contribution). We believe that the (slightly) different nature of the main NIR-transitions involved for every radical-cationic isomer could be one of the origins of the different widths for the two observed bands. Assuming the existence of roughly only one isomer in the equilibrium in DMF solution (Figure 6), the TD calculation for the COSMO/RI-BP86/Def2-TZVP optimized $[\mathbf{3}\boldsymbol{qC_s}]^{+\bullet}$ structure predicts the occurrence of only one (a bit less intense, $f$=0.0969) band at λ=1073.4 nm, now corresponding to roughly equal contributions of transitions from βHOMO-3 and βHOMO to βLUMO. In the case of the singly-bridged radical-cation $\mathbf{6}^{\bullet+}$ only one configurational isomer is possible (although displaying a complex conformational dynamics), and only one transition is expected to occur in the NIR in $CH_2Cl_2$ solution (λ=1008.9 nm, $f$=0.2840), at the same level of theory, again having βHOMO→βLUMO nature.

**Calculated structures.** Cartesian coordinates and energies computed for compound **3** and oxidized species $\mathbf{3}^{\bullet+}$.

Compound $\mathbf{3}^{\boldsymbol{Cs}}$: E = - 3486.66087122 au

$E_{chloroform}$ = -3486.667097 au

Thermal correction to G° = 0.280514 au

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 0.00000000 | 0.00000000 | 0.00000000 | C | 4.87679375 | 1.66702007 | 0.00000000 |
| Fe | 6.07261077 | 0.00000000 | 0.00000000 | C | 4.87679175 | -1.62151718 | -0.38682611 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 5.50242384 | 1.48311630 | 1.28315841 | N | 2.57295325 | 1.60482672 | 0.66848984 |
| C | 5.92658045 | -1.50269272 | -1.37107623 | N | 2.57295424 | -1.71614299 | 0.27785789 |
| C | 6.92018423 | 1.50633352 | 1.09165785 | C | 1.20905321 | 1.62360133 | 0.36469068 |
| C | 7.18327499 | -1.57220652 | -0.69063356 | C | 1.20905221 | -1.66391075 | -0.02199973 |
| C | 7.18327798 | 1.68955030 | -0.30694847 | C | 0.52435726 | 1.74551888 | -0.90606585 |
| C | 6.92018623 | -1.71853573 | 0.71231271 | C | 0.19812422 | -1.77230427 | 1.00003020 |
| C | 5.92658645 | 1.77983152 | -0.98495338 | C | -0.88452445 | 1.71881558 | -0.65237423 |
| C | 5.50242685 | -1.74038894 | 0.90397875 | C | -1.08512743 | -1.69130373 | 0.37712803 |
| H | 4.96463329 | 1.34194276 | 2.21466152 | C | -1.08512743 | 1.55763820 | 0.75927354 |
| H | 5.78069305 | -1.38639987 | -2.44165268 | C | -0.88452846 | -1.52053050 | -1.03339102 |
| H | 7.67001872 | 1.37992885 | 1.86727474 | C | 0.19812123 | 1.49189103 | 1.38397393 |
| H | 8.16387530 | -1.50379995 | -1.15253079 | C | 0.52435125 | -1.48764028 | -1.28635992 |
| H | 8.16388028 | 1.73019293 | -0.77210844 | H | 0.98524375 | 1.85180189 | -1.88353137 |
| H | 7.67002373 | -1.77556346 | 1.49608813 | H | 0.40975876 | -1.88977187 | 2.05821771 |
| H | 5.78070305 | 1.91514026 | -2.05329306 | H | -1.66703280 | 1.78741565 | -1.40311705 |
| H | 4.96463929 | -1.81922460 | 1.84281745 | H | -2.04581764 | -1.73063810 | 0.88220116 |
| C | 3.44666133 | 1.66740920 | -0.27923514 | H | -2.04582063 | 1.47870630 | 1.25968493 |
| C | 3.44665833 | -1.55709918 | -0.65852374 | H | -1.66704081 | -1.41305965 | -1.77955960 |
| H | 3.16822159 | 1.73342207 | -1.34708346 | H | 0.40975077 | 1.36061551 | 2.44053828 |
| H | 3.16821359 | -1.37351510 | -1.71254059 | H | 0.98523375 | -1.36421807 | -2.26181245 |

Compound **3**$^{C2}$: E = - 3486.66322068 au

$E_{chloroform}$ = -3486.668216 au

Thermal correction to Gº = 0.283221 au

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 0.00000000 | 0.00000000 | 0.00000000 | H | 3.34654100 | 1.81686645 | 1.53541474 |
| Fe | 6.04768500 | 0.00000000 | 0.00000000 | H | 3.34654100 | -1.81686645 | -1.53541474 |
| C | 4.88584400 | 1.69040734 | 0.00000000 | N | 2.51972500 | 1.66021061 | -0.39072786 |
| C | 4.88584400 | -1.69040734 | 0.00000000 | N | 2.51972500 | -1.66021061 | 0.39072786 |
| C | 6.04857200 | 1.85947844 | 0.83902406 | C | 1.21239299 | 1.63866444 | 0.09556571 |
| C | 6.04857200 | -1.85947844 | -0.83902406 | C | 1.21239299 | -1.63866444 | -0.09556571 |
| C | 7.21292300 | 1.68875209 | 0.02754330 | C | 0.06786700 | 1.89242980 | -0.74850363 |
| C | 7.21292300 | -1.68875209 | -0.02754330 | C | 0.06786700 | -1.89242980 | 0.74850363 |
| C | 6.78400700 | 1.39960423 | -1.30935651 | C | -1.11395600 | 1.72804989 | 0.03641883 |
| C | 6.78400700 | -1.39960423 | 1.30935651 | C | -1.11395600 | -1.72804989 | -0.03641883 |
| C | 5.35530700 | 1.39316659 | -1.32964921 | C | -0.72054700 | 1.35058142 | 1.36248200 |
| C | 5.35530700 | -1.39316659 | 1.32964921 | C | -0.72054700 | -1.35058142 | -1.36248200 |
| H | 6.03339700 | 2.07124250 | 1.90480236 | C | 0.70874000 | 1.28802085 | 1.40716304 |
| H | 6.03339700 | -2.07124250 | -1.90480236 | C | 0.70874000 | -1.28802085 | -1.40716304 |
| H | 8.24215801 | 1.73883519 | 0.37099168 | H | 0.12667700 | 2.15723352 | -1.79979440 |
| H | 8.24215801 | -1.73883519 | -0.37099168 | H | 0.12667700 | -2.15723352 | 1.79979440 |
| H | 7.43485200 | 1.19108345 | -2.15374170 | H | -2.13517200 | 1.83829841 | -0.31685660 |
| H | 7.43485200 | -1.19108345 | 2.15374170 | H | -2.13517200 | -1.83829841 | 0.31685660 |
| H | 4.71115600 | 1.19154840 | -2.17929828 | H | -1.39356500 | 1.12062734 | 2.18399846 |
| H | 4.71115600 | -1.19154840 | 2.17929828 | H | -1.39356500 | -1.12062734 | -2.18399846 |
| C | 3.50278500 | 1.72595700 | 0.44600449 | H | 1.30411200 | 0.97152350 | 2.25825604 |
| C | 3.50278500 | -1.72595700 | -0.44600449 | H | 1.30411200 | -0.97152350 | -2.25825604 |

Compound **3**$^{TS}$: E = - 3486.64375362 au

$E_{chloroform}$ = -3486.649378 au

Thermal correction to Gº = 0.282244 au

$\nu$ = -208.2 $cm^{-1}$

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Fe | 0.00000000 | 0.00000000 | 0.00000000 | H | 2.84621625 | 0.29561154 | 0.16986609 |
| Fe | 5.94877714 | 0.00000000 | 0.00000000 | H | 3.40261353 | -1.80994523 | -1.78513663 |
| C | 4.61682210 | 1.57488751 | 0.00000000 | N | 2.27713991 | 2.26357575 | 0.26931610 |
| C | 4.92148957 | -1.77679736 | -0.22673220 | N | 2.54588740 | -1.82461777 | 0.13636467 |
| C | 5.56581097 | 1.71537734 | 1.06816034 | C | 0.95962952 | 1.80544619 | 0.47544076 |
| C | 6.08868236 | -1.73050736 | -1.07654628 | C | 1.25598850 | -1.63964301 | -0.36056680 |
| C | 6.87897846 | 1.75666775 | 0.49863776 | C | -0.16200372 | 2.02685052 | -0.38673500 |
| C | 7.24056047 | -1.56902154 | -0.24634359 | C | 0.06995686 | -2.00883515 | 0.37108977 |
| C | 6.75141689 | 1.64055760 | -0.92261663 | C | -1.33184531 | 1.51842060 | 0.26604512 |
| C | 6.79911493 | -1.49234052 | 1.11569514 | C | -1.06829752 | -1.68090177 | -0.42976817 |
| C | 5.35924933 | 1.51225262 | -1.23436073 | C | -0.93573461 | 0.97010797 | 1.53040558 |
| C | 5.37378866 | -1.60324849 | 1.13236987 | C | -0.60314110 | -1.05703128 | -1.63502372 |
| H | 5.31899896 | 1.76030956 | 2.12457402 | C | 0.48200987 | 1.12403387 | 1.65145766 |
| H | 6.08346480 | -1.80530886 | -2.16065718 | C | 0.82705051 | -1.01175610 | -1.59050774 |
| H | 7.80962642 | 1.84246919 | 1.05196764 | H | -0.11643901 | 2.49900526 | -1.36351350 |
| H | 8.26813992 | -1.49098238 | -0.58944802 | H | 0.07142380 | -2.48163739 | 1.34826266 |
| H | 7.56710509 | 1.62830740 | -1.63973396 | H | -2.34049175 | 1.52772331 | -0.13734894 |
| H | 7.43651721 | -1.34510720 | 1.98284337 | H | -2.10763216 | -1.84072409 | -0.15693241 |
| H | 4.92864494 | 1.39797557 | -2.22473993 | H | -1.59113640 | 0.49960003 | 2.25782972 |
| H | 4.72293593 | -1.56669514 | 1.99994302 | H | -1.22972604 | -0.65973106 | -2.42888036 |
| C | 3.16519416 | 1.34458858 | 0.14944956 | H | 1.10433672 | 0.81370124 | 2.48589536 |
| C | 3.54747698 | -1.82904282 | -0.68957454 | H | 1.47397860 | -0.57015259 | -2.34311223 |

Compound $[\mathbf{3}^{qCs}]^{\cdot+}$: E = -3486.44246395 au

$E_{dichloromethane}$ = -3486.500976 au

$E_{DMF}$ = -3491.245903 au

Thermal correction to Gº = 0.281634 au

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 | C | -0.72449371 | -0.99428080 | -3.55013730 |
| C | 1.44234959 | 0.00000000 | 0.00000000 | H | -0.21295165 | -1.97210283 | -3.55959333 |
| C | 1.87587533 | 1.35985337 | 0.00000000 | N | -2.01529974 | -0.87014799 | -3.60825840 |
| C | 0.71398208 | 2.20121414 | -0.02252123 | C | -2.92148255 | -2.20570220 | -0.22621435 |
| C | -0.44629333 | 1.36984101 | -0.04114608 | C | -4.35530586 | -2.11278813 | -0.33044529 |
| H | 2.08032911 | -0.87895217 | 0.01491731 | C | -4.87445024 | -3.43151748 | -0.49231838 |
| H | 2.90745545 | 1.69820726 | -0.00342522 | C | -3.77129713 | -4.34703794 | -0.51998248 |
| H | 0.71800851 | 3.28668410 | -0.04770472 | C | -2.56010083 | -3.60054410 | -0.38337848 |
| H | -1.48370110 | 1.68492200 | -0.07134123 | H | -4.91563594 | -1.18487358 | -0.27917543 |
| Fe | 0.74092451 | 0.97753425 | -1.67299256 | H | -5.92238376 | -3.69582958 | -0.59458146 |
| C | 0.12954020 | 0.17419025 | -3.48467381 | H | -3.84079440 | -5.42382137 | -0.64318865 |
| C | -0.30747052 | 1.54068515 | -3.35040267 | H | -1.56033204 | -4.02269830 | -0.37016517 |
| C | 0.85691558 | 2.35195956 | -3.19656584 | Fe | -3.60095297 | -2.98340208 | -2.04507161 |
| C | 2.01021482 | 1.49862912 | -3.20584152 | C | -2.81841898 | -1.99623851 | -3.71455215 |
| C | 1.56746826 | 0.15155336 | -3.36888713 | C | -2.47662978 | -3.40456765 | -3.71479329 |
| H | -1.34141369 | 1.86762173 | -3.37277916 | C | -3.69873240 | -4.14502515 | -3.73550566 |
| H | 0.86743593 | 3.43001081 | -3.06774519 | C | -4.79205728 | -3.21779037 | -3.70574578 |
| H | 3.04074862 | 1.81923589 | -3.08806269 | C | -4.25509123 | -1.89649190 | -3.67533817 |
| H | 2.19765982 | -0.73182331 | -3.41668009 | H | -1.48067333 | -3.83557276 | -3.73162036 |
| C | -0.83811772 | -1.17655501 | -0.11164699 | H | -3.78270890 | -5.22766772 | -3.75209301 |
| H | -0.31435459 | -2.14747290 | -0.14039994 | H | -5.84589373 | -3.47801686 | -3.69219579 |
| N | -2.13112774 | -1.06801893 | -0.15419372 | H | -4.80502077 | -0.96160859 | -3.64046277 |

Compound $[\mathbf{3}^{C2}]^{\cdot+}$: E = - 3486.44332539 au

$E_{dichloromethane}$ = -3486.500147 au

$E_{DMF}$ = -3491.239041 au

Thermal correction to Gº = 0.281443 au

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 | C | -1.48041304 | -0.11379071 | -3.55843913 |
| C | 1.43864449 | 0.00000000 | 0.00000000 | H | -2.36721491 | 0.54013930 | -3.59182022 |
| C | 1.87691608 | 1.35756764 | 0.00000000 | N | -1.55529406 | -1.40966747 | -3.60821977 |
| C | 0.72110674 | 2.20388538 | -0.01283894 | C | -2.93028792 | -2.18895120 | -0.21949120 |
| C | -0.44095379 | 1.37786649 | -0.03655652 | C | -4.36540508 | -2.08856427 | -0.21198735 |
| H | 2.07493666 | -0.88042254 | -0.00633882 | C | -4.90513715 | -3.39169157 | -0.41562341 |
| H | 2.91024642 | 1.69066393 | -0.01694112 | C | -3.81602007 | -4.30866508 | -0.57573374 |
| H | 0.73023248 | 3.28954302 | -0.03381217 | C | -2.59127514 | -3.57692238 | -0.48554202 |
| H | -1.47669161 | 1.70002710 | -0.05000356 | H | -4.91487667 | -1.16320114 | -0.07129524 |
| Fe | 0.72566126 | 0.98153327 | -1.67494753 | H | -5.96008448 | -3.64346284 | -0.46452181 |
| C | -0.19407640 | 0.54540777 | -3.48027400 | H | -3.90412680 | -5.37531587 | -0.76048740 |
| C | 0.01250019 | 1.96314977 | -3.34970760 | H | -1.59621275 | -3.99937830 | -0.58172623 |
| C | 1.41330357 | 2.19034299 | -3.20402668 | Fe | -3.72672460 | -2.85513664 | -2.02795633 |
| C | 2.08020295 | 0.92271541 | -3.23011421 | C | -2.79189923 | -2.02941273 | -3.69916225 |
| C | 1.09715911 | -0.09976202 | -3.37647416 | C | -2.89835784 | -3.45823262 | -3.82889745 |
| H | -0.76434362 | 2.72245524 | -3.35436737 | C | -4.27852009 | -3.80955517 | -3.77746223 |
| H | 1.88841161 | 3.15710354 | -3.06743342 | C | -5.04030542 | -2.61050891 | -3.59139068 |
| H | 3.14951008 | 0.76637417 | -3.12374990 | C | -4.13515324 | -1.50683634 | -3.51271944 |
| H | 1.26469054 | -1.17007637 | -3.43198406 | H | -2.05257806 | -4.12825358 | -3.94610795 |
| C | -0.84142105 | -1.17436652 | -0.09048838 | H | -4.68254500 | -4.81503997 | -3.84423700 |
| H | -0.32736608 | -2.14950060 | -0.08649727 | H | -6.12086509 | -2.55094496 | -3.49928548 |
| N | -2.13373398 | -1.05664878 | -0.14924963 | H | -4.41731659 | -0.47004573 | -3.36001582 |

Compound $[\mathbf{3}^{TS}]^{+}$: E = -3486.42338533 au

$E_{dichloromethane}$ = -3486.481216 au

$E_{DMF}$ = -3491.206022 au

Thermal correction to Gº = 0.282887 au

$\nu$ = -192.2 $cm^{-1}$

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 | C | -1.30130237 | -0.54879633 | -3.43031194 |
| C | 1.44173245 | 0.00000000 | 0.00000000 | H | -1.61310613 | -0.89274113 | -2.43476605 |
| C | 1.88428428 | 1.35567486 | 0.00000000 | N | -1.94810685 | -0.95021318 | -4.45761661 |
| C | 0.72917707 | 2.20352140 | -0.01808211 | C | -2.90340555 | -2.16992744 | -0.56406847 |
| C | -0.43520107 | 1.37796805 | -0.04967884 | C | -4.33932784 | -2.07938787 | -0.59983504 |
| H | 2.07628643 | -0.88185454 | 0.00104189 | C | -4.86361186 | -3.37972557 | -0.86092703 |
| H | 2.91834591 | 1.68657715 | -0.00505882 | C | -3.76171999 | -4.27380413 | -1.06008175 |
| H | 0.73772489 | 3.28924816 | -0.03160167 | C | -2.54802333 | -3.52783617 | -0.92532064 |
| H | -1.47031535 | 1.70215483 | -0.07221186 | H | -4.90119999 | -1.17067231 | -0.40865446 |
| Fe | 0.74361046 | 0.99445263 | -1.67873096 | H | -5.91554487 | -3.64205864 | -0.91847256 |
| C | -0.14439882 | 0.36903135 | -3.46202765 | H | -3.83165215 | -5.33235454 | -1.29270777 |
| C | -0.20060803 | 1.79444235 | -3.34750488 | H | -1.54489582 | -3.92965559 | -1.02997022 |
| C | 1.14080988 | 2.27999076 | -3.23563533 | Fe | -3.71966974 | -2.78081522 | -2.46202670 |
| C | 2.02855199 | 1.15823239 | -3.27069118 | C | -2.99548759 | -1.84497899 | -4.26630197 |
| C | 1.23897089 | -0.02993597 | -3.39084801 | C | -2.87926543 | -3.27132268 | -4.31681201 |
| H | -1.10626197 | 2.39283028 | -3.33368904 | C | -4.18985616 | -3.82467473 | -4.15956821 |
| H | 1.42930310 | 3.32120121 | -3.12822152 | C | -5.10899217 | -2.74393057 | -3.96094279 |
| H | 3.11158309 | 1.19650124 | -3.20450323 | C | -4.36718236 | -1.51821435 | -3.98791715 |
| H | 1.61115300 | -1.04812949 | -3.44866498 | H | -1.95800928 | -3.81816813 | -4.49171533 |
| C | -0.83900075 | -1.17124842 | -0.10796122 | H | -4.43840750 | -4.88145250 | -4.17722435 |
| H | -0.34092816 | -2.15035366 | -0.00533680 | H | -6.17977453 | -2.83394024 | -3.80529253 |
| N | -2.11598084 | -1.05451536 | -0.34325250 | H | -4.76478166 | -0.51403326 | -3.87975530 |