Diarylferrocene Tweezers for Cation Binding

(Supplementary Information)

Carlos F. R. A. C. Lima,*[a,b] Ana M. Fernandes,[b] André Melo,[c] Luís M. Gonçalves,[c] Artur M. S. Silva[b] and Luís M. N. B. F. Santos*[a]

[a] CIQ, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, P-4169-007 Porto, Portugal.

[b] Department of Chemistry & QOPNA, University of Aveiro, P-3810-193 Aveiro, Portugal.

[c] REQUIMTE, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, P-4169-007 Porto, Portugal.

* Corresponding authors:

Carlos F. R. A. C. Lima, Luís M. N. B. F. Santos
CIQ, Departamento de Química e Bioquímica, Faculdade de Ciências da Universidade do Porto, P-4169-007 Porto, Portugal.
E-mail: carlos.chemistry@gmail.com, lbsantos@fc.up.pt

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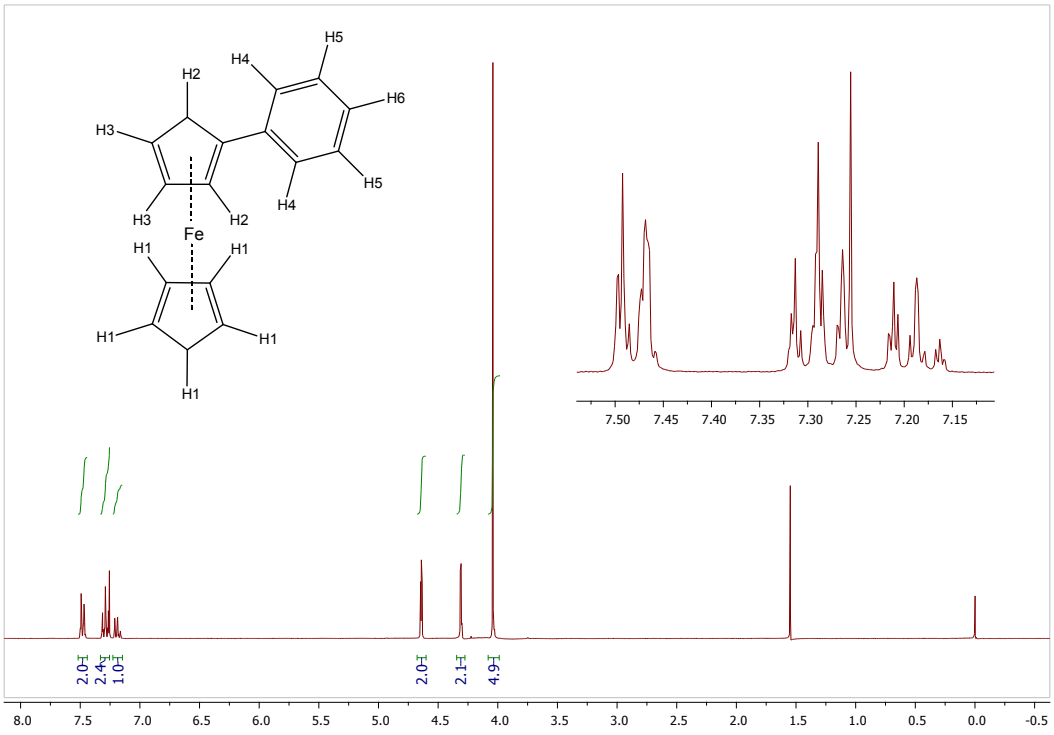
Section S1. Synthesis and characterization

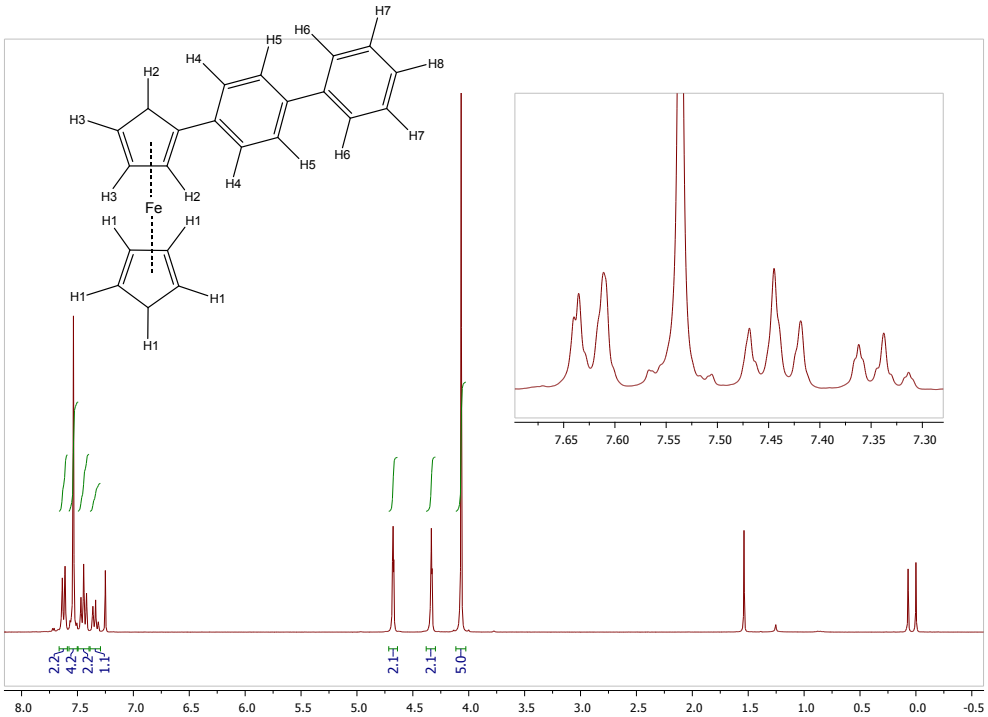
1.1. General remarks. Ferrocene, 1-bromoferrocene, 1,1'-dibromoferrocene, all the boronic acids, and $Pd(OAc)_2$ were commercially obtained from Sigma-Aldrich. The ^1H and ^{13}C NMR spectra in solution were recorded on a Bruker Avance 300 spectrometer (300.13 MHz), using TMS as internal reference and $CDCl_3$ as the solvent. Reaction yields (%) are calculated from the mass of isolated product obtained, corrected for the sample %(*m*/*m*) purity. All purity analyses were made by GC, using an HP 4890 apparatus equipped with an HP-5 column, cross-linked, 5% diphenyl and 95% dimethylpolysiloxane. ^1H NMR data is given as: chemical shift (number of protons, multiplicity, atom numbering/identification, coupling constant).

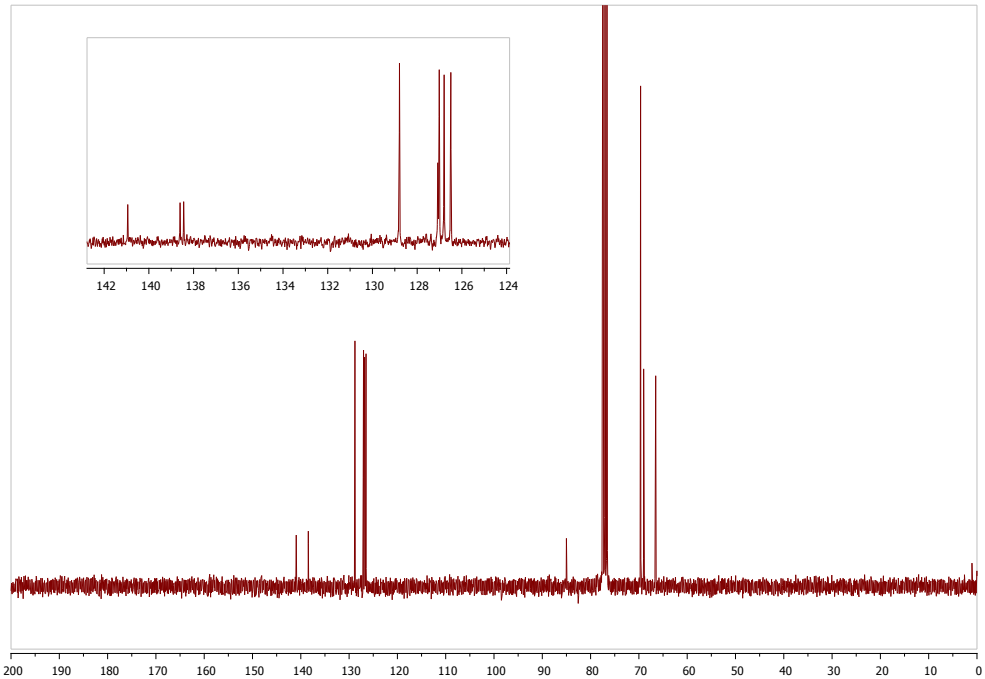
1.2. General synthesis of 1-arylferrocenes (**1a−d**). A solution of K_2CO_3 (1.4 mol/equiv) in 12 ml of water per 1 mmol of the limiting reactant was added to a solution of 1-bromoferrocene (1 mol/equiv), arylboronic acid (1.2 mol/equiv) and Pd(OAc)2 (2 mol %) in the same volume of DMF. The resultant mixture was heated at 80 ºC for 5 h under stirring. The final solution was allowed to cool to room temperature and extracted with dichloromethane or ethyl acetate. The organic layer was washed with water and aqueous 0.1 M KOH, dried over anhydrous sodium sulfate and evaporated, yielding the product as impure 1-arylferrocene.

1.2.1. *1-Phenylferrocene,* ***1a*** *(R = H)*. The orange oil obtained (0.36 g, η = 46%) was washed with MeOH and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.51-7.45 (2H, m, H4), 7.29 (2H, t, H5, J = 7.2 Hz), 7.19 (1H, tt, H6, J_1 = 7.2 Hz, J_2 = 1.6 Hz), 4.65 (2H, t, H2, J = 1.8 Hz), 4.31 (2H, t, H3, J = 1.8 Hz), 4.04 (5H, s, H1); see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 262.0, found 262.0.

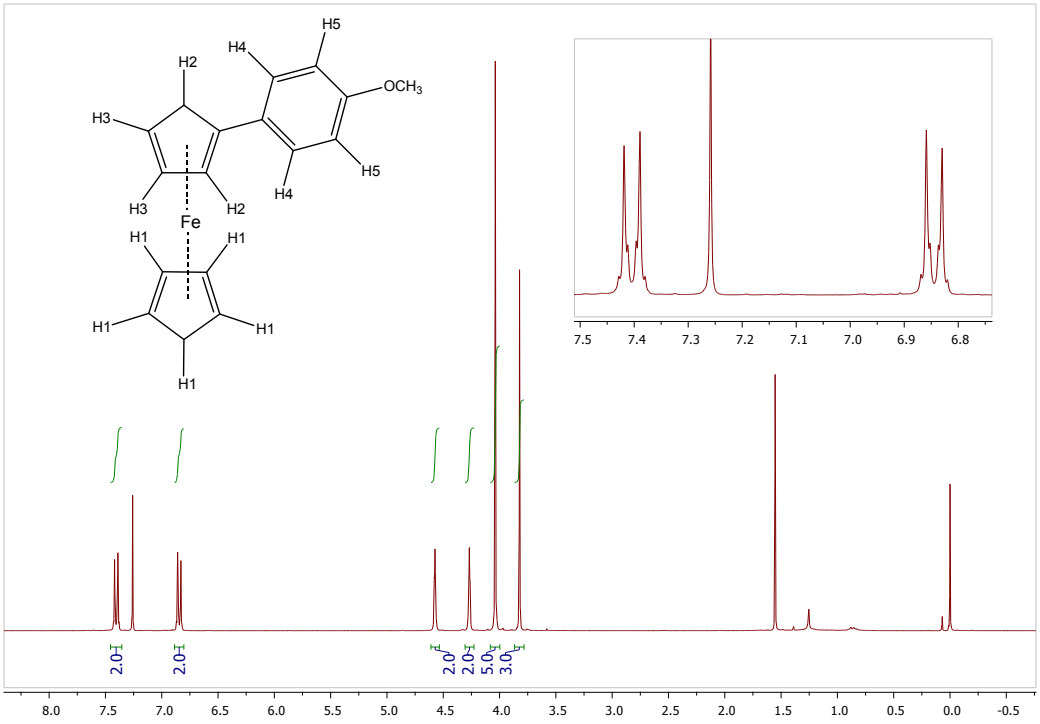


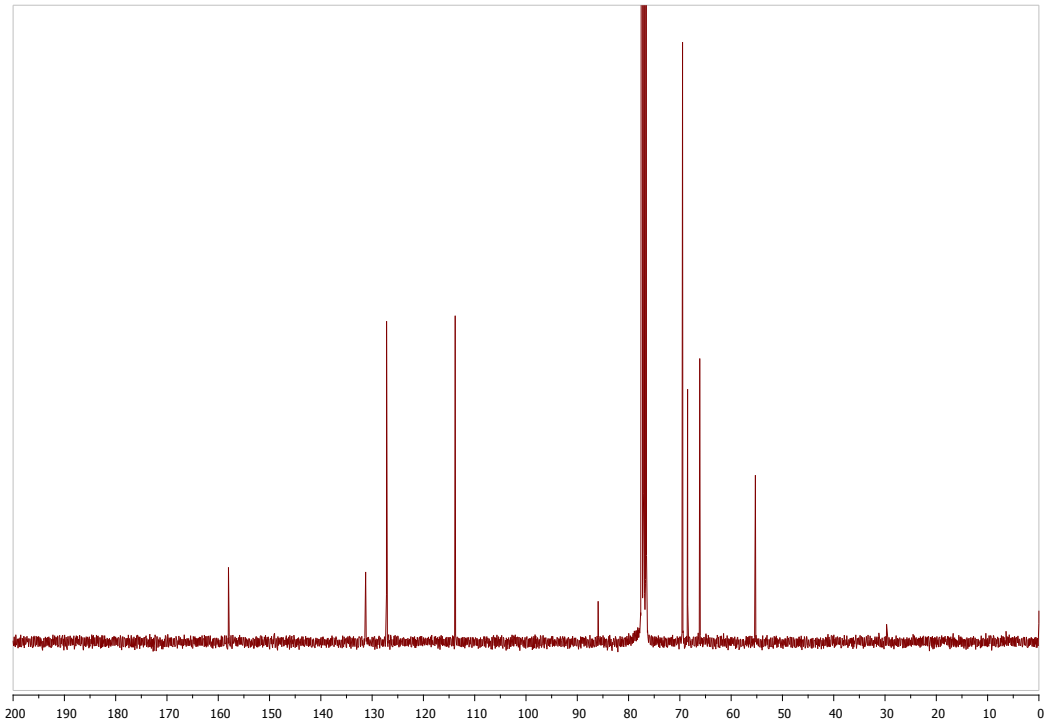
1.2.2. *1-([1,1'-Biphenyl]-4-yl)ferrocene* ***1b*** *(R = Ph)*. The orange flakes obtained (0.27 g, η = 53%) were washed with MeOH and diethyl ether and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.62 (2H, d, H6, *J* = 7.2 Hz), 7.54 (4H, m, H4 + H5), 7.44 (2H, t, H7, *J* = 7.3 Hz), 7.34 (1H, t, H8, *J* = 7.3 Hz), 4.68 (2H, t, H2, *J* = 1.8 Hz), 4.33 (2H, t, H3, *J* = 1.8 Hz), 4.07 (5H, s, H1); ^{13}C NMR (75.47 MHz, $CDCl_3$): 140.9, 138.6, 138.4, 128.8, 127.1, 127.0, 126.8, 126.5, 85.0, 69.6, 69.0, 66.5; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 338.1, found 338.1.



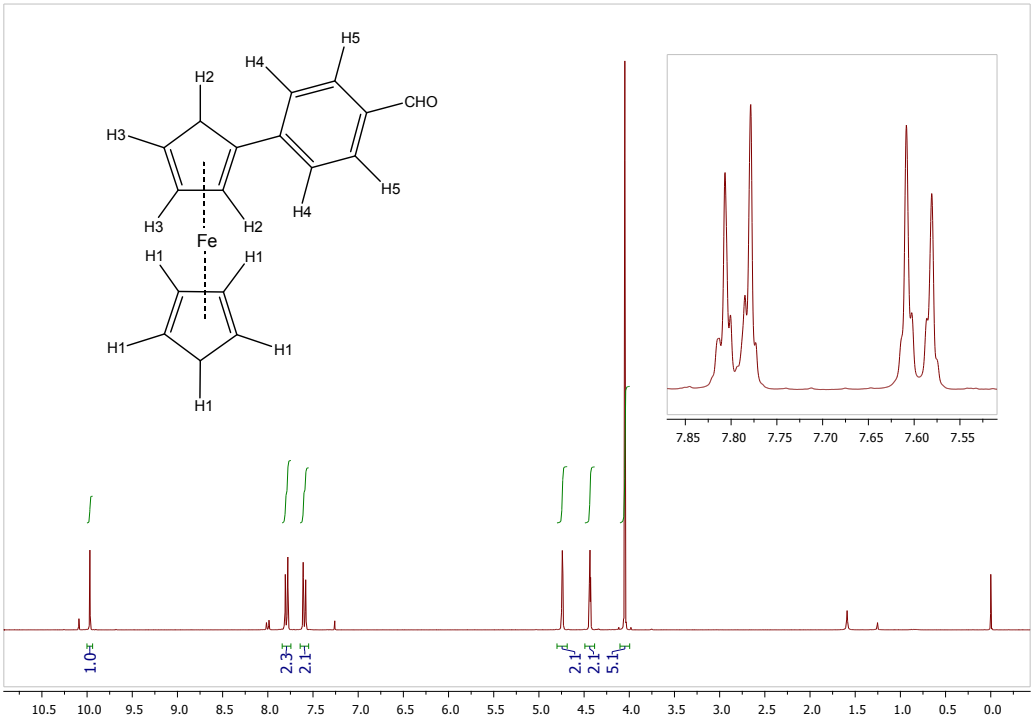


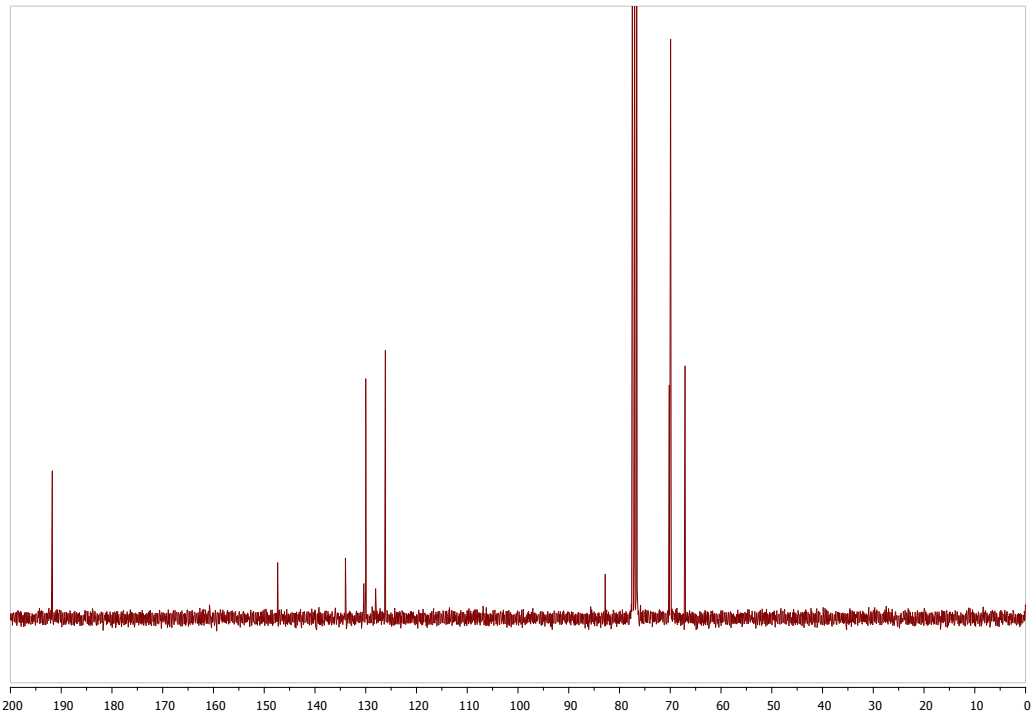
1.2.3. *1-(4-Methoxyphenyl)ferrocene* ***1c*** *(R = OCH_3)*. The orange oil obtained (0.27 g, η = 46%) was washed with MeOH and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.40 (2H, dt, H4, J_1 = 8.7 Hz, J_2 = 2.5 Hz), 6.84 (2H, dt, H5, J_1 = 8.7 Hz, J_2 = 2.5 Hz), 4.57 (2H, t, H2, J = 1.8 Hz), 4.27 (2H, t, H3, J = 1.8 Hz), 4.04 (5H, s, H1), 3.82 (3H, s, OCH_3); ^{13}C NMR (75.47 MHz, $CDCl_3$): 158.0, 131.3, 127.2, 113.8, 85.9, 69.5, 68.5, 66.1, 55.3; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 292.1, found 292.1.





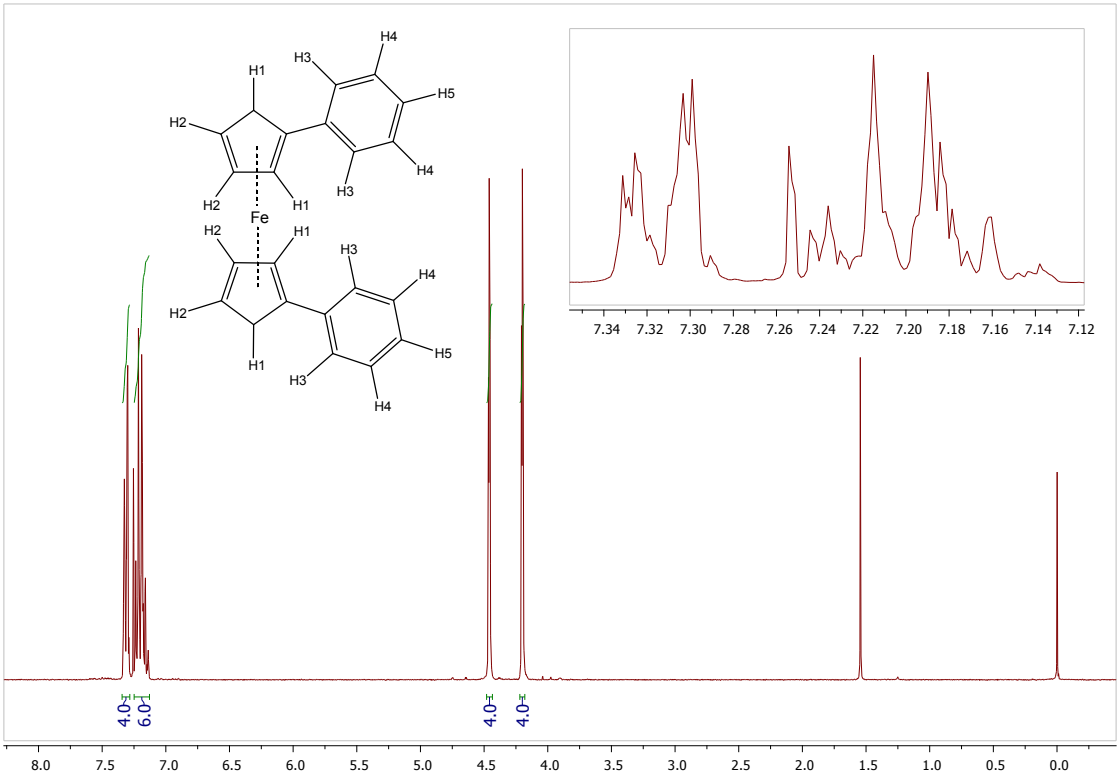
1.2.4. *4-(Ferrocen-1-yl)benzaldehyde* ***1d*** *(R = CHO)*. The orange oil obtained (0.19 g, η = 33%) was washed with MeOH and sublimed under reduced pressure to yield dark orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 9.97 (1H, s, CHO), 7.79 (2H, d, H5, J = 8.4), 7.59 (2H, d, H4, J = 8.4 Hz), 4.74 (2H, t, H2, J = 1.8 Hz), 4.44 (2H, t, H3, J = 1.8 Hz), 4.05 (5H, s, H1); ^{13}C NMR (75.47 MHz, $CDCl_3$): 191.8, 147.4, 134.0, 130.0, 126.1, 82.8, 70.2, 69.9, 67.1; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 290.0, found 290.0.



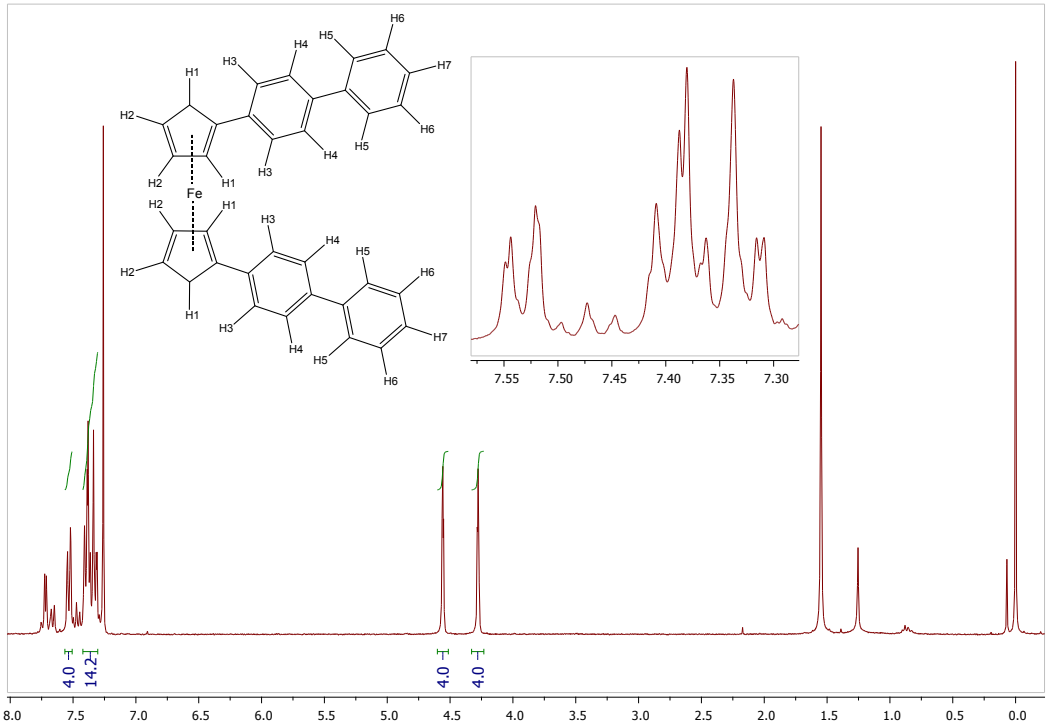


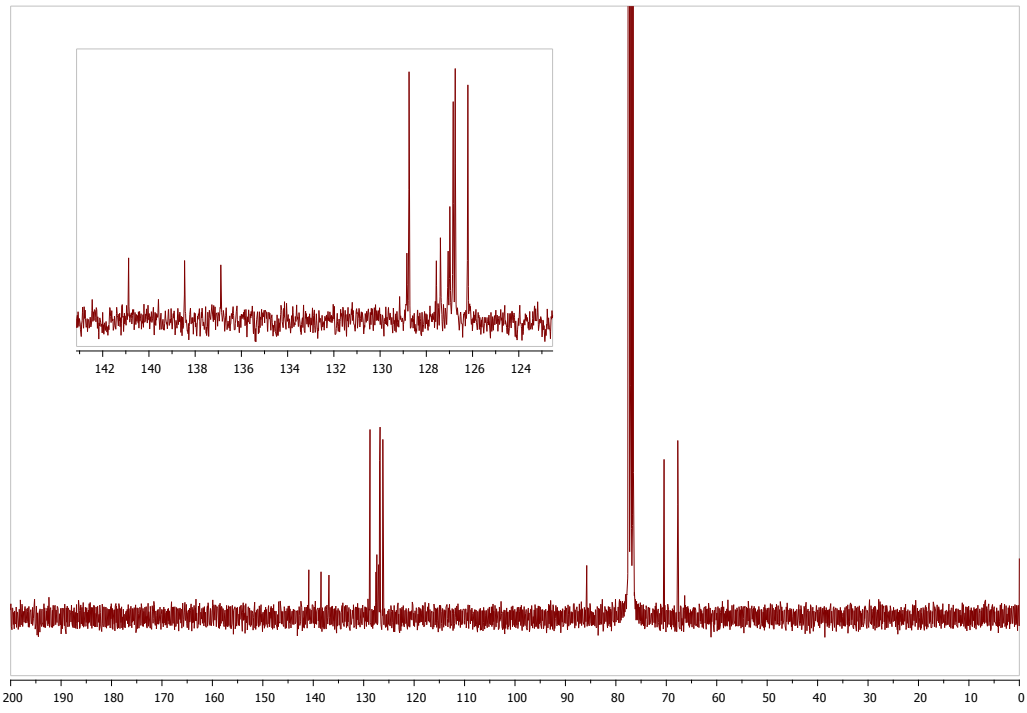
1.3. General synthesis of 1,1'-diarylferrocenes (**2a–d**). A solution of K_2CO_3 (6 mol/equiv) in 15 ml of water per 1 mmol of the limiting reactant was added to a solution of 1,1'-dibromoferrocene (1 mol/equiv), arylboronic acid (4 mol/equiv) and $Pd(OAc)_2$ (2 mol %) in the same volume of DMF. The resultant mixture was heated at 80 ºC for 5 h under stirring. The final solution was allowed to cool to room temperature and extracted with dichloromethane. The organic layer was washed with water and aqueous 0.1 M KOH, dried over anhydrous sodium sulfate and evaporated, yielding the product as impure 1,1'-diarylferrocene.

1.3.1. *1,1'-Diphenylferrocene* ***2a*** *(R = H)*. The orange powder obtained (0.20 g, η = 59%) was washed with MeOH and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.34–7.29 (4H, m, H3), 7.25–7.13 (6H, m, H4 + H5), 4.46 (4H, t, H1, J = 1.8 Hz), 4.20 (4H, t, H2, J = 1.8 Hz); see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 338.1, found 338.0.

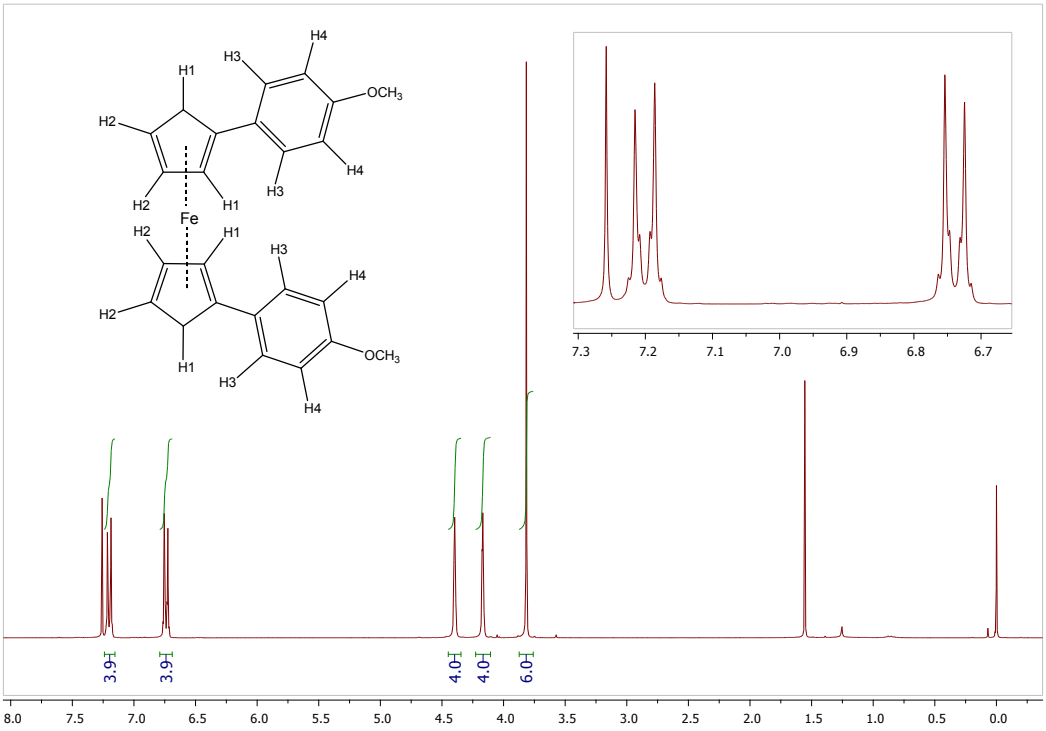


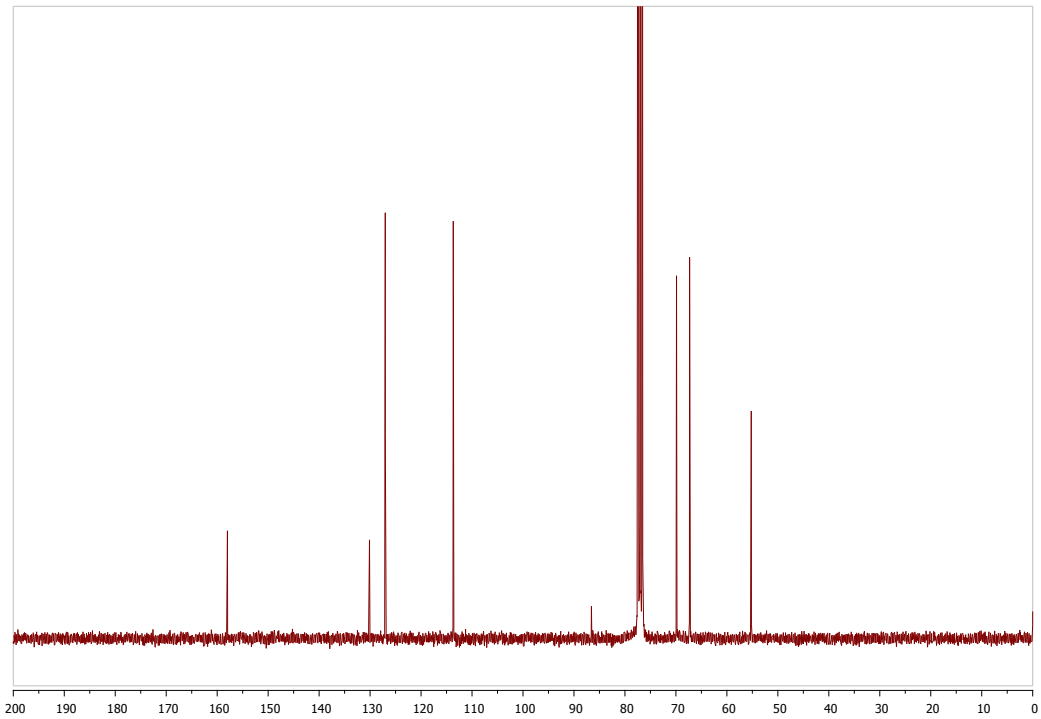
1.3.2. *1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene* ***2b*** *(R = Ph)*. The orange powder obtained (0.13 g, η = 27%) was washed with MeOH and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.53 (4H, d, H5, J = 6.9 Hz), 7.42−7.30 (14H, m, H3 + H4 + H6 + H7), 4.56 (4H, t, H1, J = 1.8 Hz), 4.28 (4H, t, H2, J = 1.8 Hz); ^{13}C NMR (75.47 MHz, $CDCl_3$): 140.9, 138.5, 136.9, 128.7, 127.0, 126.8, 126.7, 126.2, 85.8, 70.4, 67.7; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 490.1, found 490.1.



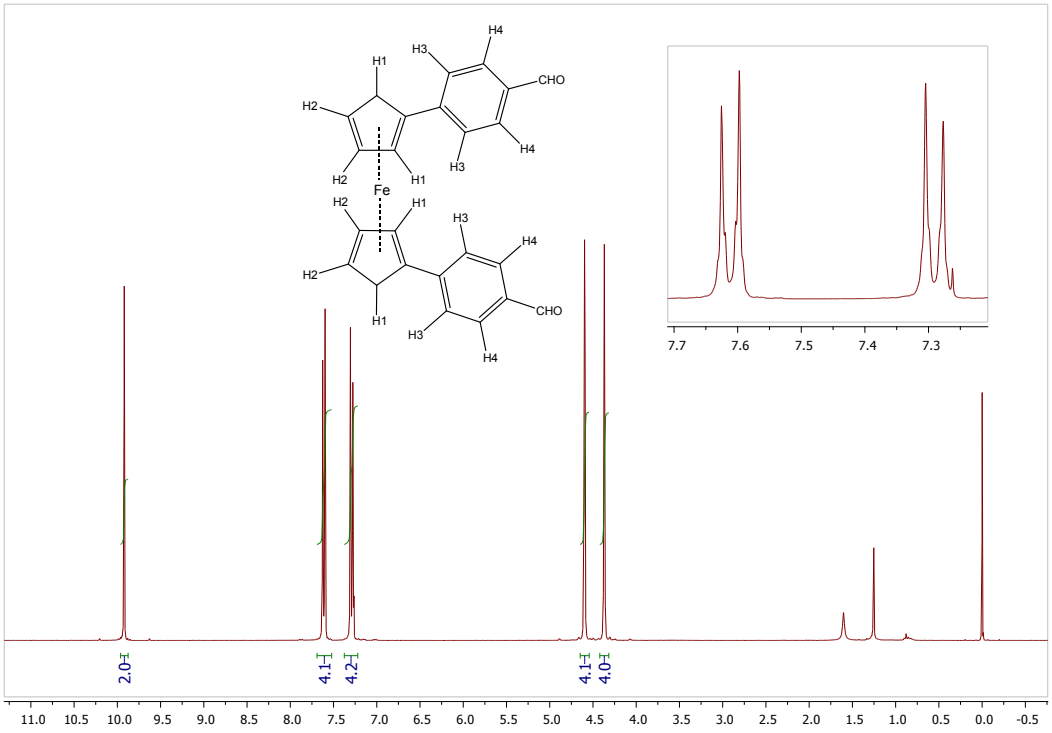


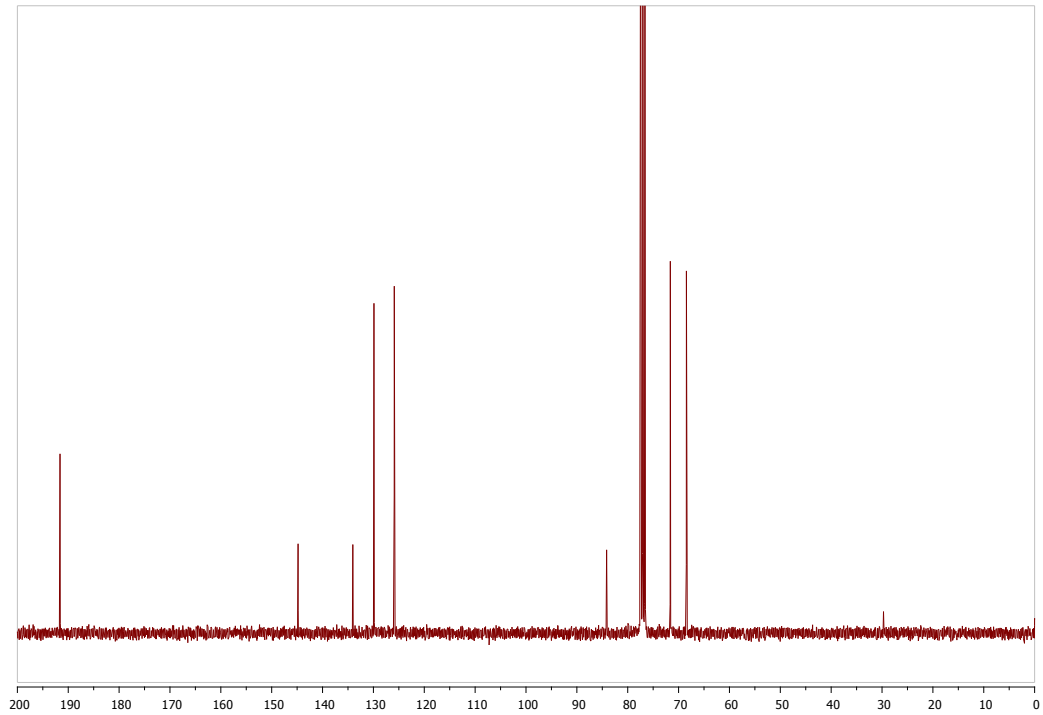
1.3.3. *1,1'-Bis(4-methoxyphenyl)ferrocene* ***2c*** *($R = OCH_3$)*. The orange powder obtained (0.17 g, η = 49%) was washed with MeOH and sublimed under reduced pressure to yield orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 7.20 (4H, dt, H3, J_1 = 8.7 Hz, J_2 = 2.5 Hz), 6.74 (4H, dt, H4, J_1 = 8.7 Hz, J_2 = 2.5 Hz), 4.40 (4H, t, H1, J = 1.8 Hz), 4.17 (4H, t, H2, J = 1.8 Hz), 3.82 (6H, s, OCH_3); ^{13}C NMR (75.47 MHz, $CDCl_3$): 158.0, 130.1, 127.0, 113.7, 86.6, 69.9, 67.3, 55.2; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 398.1, found 398.1.





1.3.4. *4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde* ***2d*** *(R = CHO)*. The orange powder obtained (0.16 g, η = 41%) was washed with MeOH and sublimed under reduced pressure to yield dark orange crystals of the titled compound; ^{1}H NMR (300.13 MHz, $CDCl_3$): 9.92 (2H, s, CHO), 7.61 (4H, d, H4, *J* = 8.4 Hz), 7.29 (4H, d, H3, *J* = 8.4 Hz), 4.60 (4H, t, H1, *J* = 1.8 Hz), 4.37 (4H, t, H2, *J* = 1.8 Hz); ^{13}C NMR (75.47 MHz, $CDCl_3$): 191.6, 144.8, 134.0, 129.9, 125.9, 84.2, 71.6, 68.5; see spectrum below for atom numbering. ESI-MS: calculated for (M^+) 394.1, found 394.1.





Section S2. Mass spectrometry analysis

2.1. Electrospray Ionization mass spectra of 1-arylferrocenes (**1a-d**) and 1,1'-diarylferrocenes (**2a-d**)

As an illustration, figure S1 represents the ESI-MS spectrum of 4,4'-(ferrocen-1,1'-diyl)dibenzaldehyde, **2d** (R = CHO), in the positive mode (+).

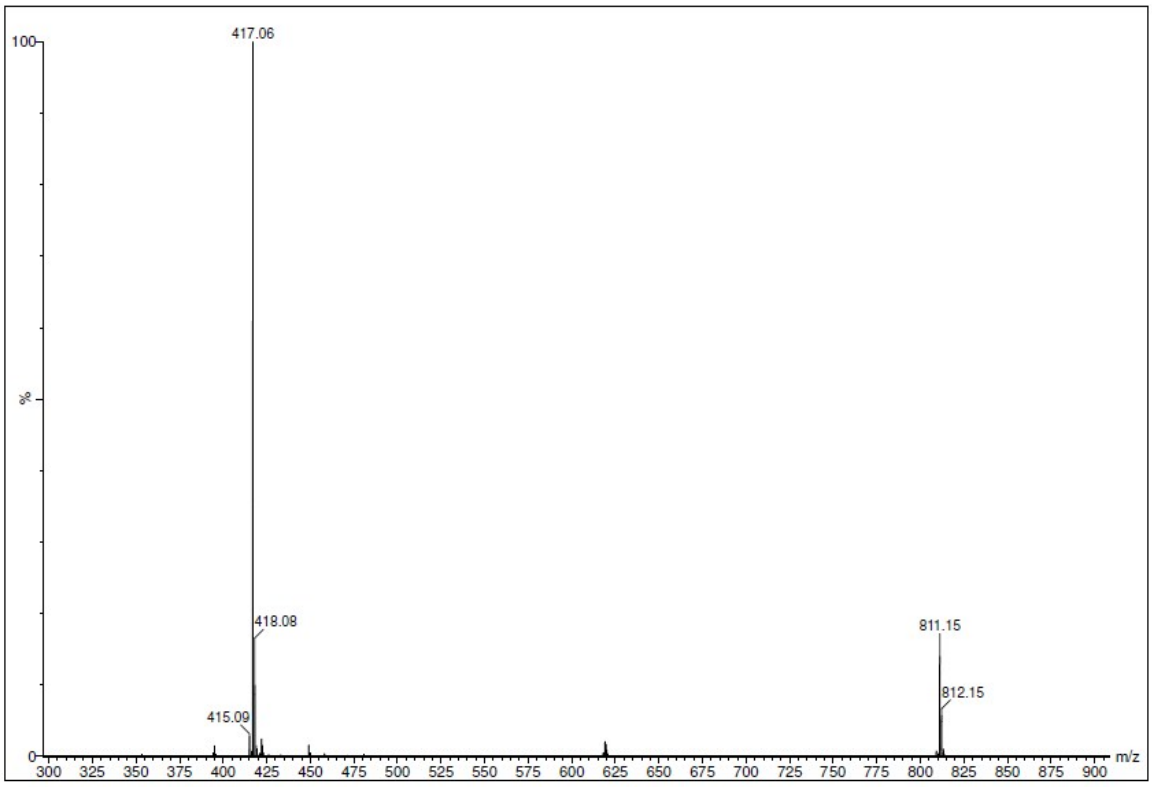


Figure S1. ESI-MS(+) of 4,4'-(ferrocen-1,1'-diyl)dibenzaldehyde **2d**.

2.2. Electrospray ionization MS-MS spectra

Figure S2 shows, as an illustration, the ESI-MS-MS spectra of the $[2M+NH_4]^+$ ion for 4,4'-(ferrocen-1,1'-diyl)dibenzaldehyde, **2d** (R = CHO).

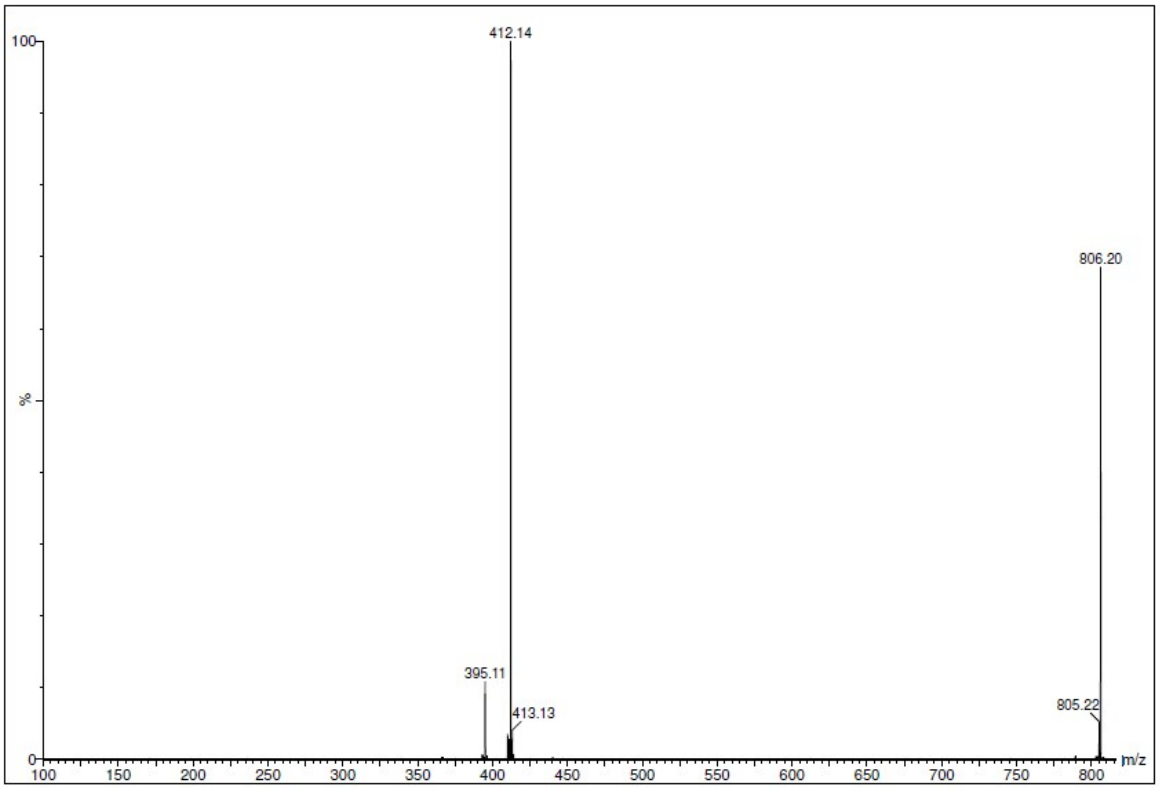


Figure S2. ESI-MS-MS spectrum of $[2M+NH_4]^+$ [M = **2d** (R = CHO)] at a collision energy of 4,0 eV.

The $E_{cm,1/2}$ values obtained for $[2M+NH_4]^+$, $[2M+Na]^+$ and $[2M+Li]^+$, M = **2d** (R = CHO), by the procedure described in the experimental part, are shown below.

	Ion m/z	$E_{Lab,1/2}$/eV	$E_{cm,1/2}$/eV
$[2M+NH_4]^+$	806	4.5	0,212
$[2M+Na]^+$	811	10.5	0.495
$[2M+Li]^+$	795	13.7	0.654

Section S3. Quantum chemistry calculations

3.1. Conformational analysis of 1,1'-diarylferrocenes (**2a-d**) in the gas phase.

Tables S1 and S2 show the results of the conformational analysis carried out by computational chemistry for the ferrocenes studied.

Table S1. Electronic energies, E_{el}, and enthalpies at T = 298.15 K, H_{298K}, ($H_{298K} = E_{el}$ + ZPE + T_cH, where ZPE and T_cH are the unscaled zero-point energy and thermal correction to enthalpy, respectively) obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory and used for the evaluation of folded/unfolded energetics.

Molecular system	E_{el} / hartree	H_{298K} / hartree
Ferrocene	−510.790210	−510.440471
1-Phenylferrocene **1a**	−741.762210	−741.243611
1-([1,1'-Biphenyl]-4-yl)ferrocene **1b**	−972.732363	−972.045020
1-(4-Methoxyphenyl)ferrocene **1c**	−856.244041	−855.656075
4-(Ferrocen-1-yl)benzaldehyde **1d**	−855.049214	−854.508910
1,1'-Diphenylferrocene (folded) **2a**	−972.738341	−972.050715
1,1'-Diphenylferrocene (unfolded) **2a**	−972.734271	−972.046880
1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene (folded) **2b**	−1434.686464	−1433.665030
1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene (unfolded) **2b**	−1434.673997	−1433.652961
1,1'-Bis(4-methoxyphenyl)ferrocene (folded) **2c**	−1201.705875	−1200.880340
1,1'-Bis(4-methoxyphenyl)ferrocene (unfolded) **2c**	−1201.697581	−1200.872451
4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde (folded) **2d**	−1199.315624	−1198.585378
4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde (unfolded) **2d**	−1199.307801	−1198.578614

Table S2. Electronic energies, E_{el}, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory, for the *syn*/*anti* conformers of **2c** (R = OCH_3) and **2d** (R = CHO).

Molecular system	E_{el} / hartree (Δ_rE_{el} / kJ·mol^{-1}) [a]
	M06-2X
1,1'-Bis(4-methoxyphenyl)ferrocene (*anti*)	−1201.705875
1,1'-Bis(4-methoxyphenyl)ferrocene (*syn*)	−1201.704198 **(4.4)**
4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde (*anti*)	−1199.315624
4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde (*syn*)	−1199.313539 **(5.5)**

[a] The Δ_rE_{el} for the *anti* → *syn* isomerization reaction is shown in parenthesis. The most stable conformer is shown in bold.

3.2. PES scans and interaction energy calculations.

Table S3. Results for the scan of the potential energy surface (PES) relative to the *d*(Fe···Na^+) degree of freedom in 1,1'-diphenylferrocene **2a**, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

d(Fe···Na^+) / Å	E_{el} / Hartree	$\Delta_{rel}E_m$ / kJ·mol^{-1}	$\Delta_{int}E_m$ / kJ·mol^{-1}
2.8	-1134.837755	58	-144
3.2	-1134.844206	41	-161
3.6	-1134.849694	26	-176
4.0	-1134.853591	16	-186
4.42	**-1134.859717**	**0**	**-202**
4.8	-1134.856105	9	-192
5.2	-1134.853981	15	-187
5.6	-1134.848286	30	-172
6.0	-1134.842916	44	-158
6.4	-1134.837926	57	-145
6.8	-1134.832557	71	-131

Table S4. Results for the scan of the potential energy surface (PES) relative to the *d*(Fe···Na^+) degree of freedom in 1,1'-bis([1,1'-diphenyl]-4-yl)ferrocene **2b**, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

d(Fe···Na^+) / Å	E_{el} / Hartree	$\Delta_{rel}E_m$ / kJ·mol^{-1}	$\Delta_{int}E_m$ / kJ·mol^{-1}
3.5	-1596.794692	38	-167
4.36	**-1596.805225**	**10**	**-195**
5.5	-1596.797344	31	-174
6.5	-1596.794281	39	-166
7.5	-1596.793856	40	-165
8.5	-1596.804585	12	-193
8.70	**-1596.809006**	**0**	**-205**
9.5	-1596.790021	50	-155
10.5	-1596.782395	70	-135

Table S5. Results for the scan of the potential energy surface (PES) relative to the *d*(Fe···Na^+) degree of freedom in 1,1'-bis(4-methoxyphenyl)ferrocene **2c**, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

d(Fe···Na^+) / Å	E_{el} / Hartree	$\Delta_{rel}E_m$ / kJ·mol^{-1}	$\Delta_{int}E_m$ / kJ·mol^{-1}
3.5	-1363.817267	25	-176
4.0	-1363.821181	14	-186
4.34	**-1363.826649**	**0**	**-200**
4.5	-1363.824898	5	-196
5.0	-1363.820908	15	-185
5.5	-1363.815277	30	-170
6.0	-1363.816340	27	-173
6.5	-1363.818285	22	-178
7.0	-1363.822309	11	-189
7.31	**-1363.826478**	**0**	**-200**
7.5	-1363.810885	41	-159
8.0	-1363.806306	53	-147
8.5	-1363.809532	45	-155
9.0	-1363.792862	89	-112
9.5	-1363.782354	116	-84
10.0	-1363.771378	145	-55
10.5	-1363.758078	180	-20

Table S6. Results for the scan of the potential energy surface (PES) relative to the $d(Fe\cdots Na^+)$ degree of freedom in 4,4'-(ferrocen-1,1'-diyl)dibenzaldehyde **2d**, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

$d(Fe\cdots Na^+)$ / Å	E_{el} / Hartree	$\Delta_{rel}E_m$ / kJ·mol^{-1}	$\Delta_{int}E_m$ / kJ·mol^{-1}
3.5	-1361.406673	123	-122
4.0	-1361.412801	107	-138
4.5	-1361.412946	107	-139
5.0	-1361.412584	108	-138
5.5	-1361.415847	99	-146
6.0	-1361.416509	97	-148
6.5	-1361.432004	57	-189
7.0	-1361.428094	67	-178
7.5	-1361.438112	41	-205
8.0	-1361.441327	32	-213
8.5	-1361.449263	11	-234
8.9	**-1361.453577**	**0**	**-245**
9.5	-1361.448903	12	-233
10.0	-1361.435144	48	-197
10.5	-1361.421736	84	-162

Table S7. Electronic energies, E_{el}, and unscaled ZPE (zero-point energy) and T_cH (thermal correction to enthalpy to 298.15 K), obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory for the systems studied, and MP2/6-31+G(d,p)/SDD(Fe) electronic energies, E_{el} (MP2), obtained from a single point energy calculation on the M06-2X/6-31+G(d,p)/SDD(Fe) optimized geometries. E_{el} for the complexes s is corrected for BSSE by the counterpoise method. All optimized geometries were obtained using M06-2X/6-31+G(d,p)/SDD(Fe).

Molecular system [a]	E_{el} / hartree	ZPE / hartree	T_cH / hartree	E_{el} (MP2) / hartree
Ferrocene	−510.790210	0.170426	0.179313	---
1a (R = H)	−741.762210	0.252570	0.266029	---
1b (R = Ph)	−972.732363	0.334154	0.353189	---
1c (R = OCH_3)	−856.244041	0.285544	0.302422	---
1d (R = CHO)	−855.049214	0.261947	0.278357	---
2a (R = H) (folded)	−972.738341	0.334461	0.353165	−969.815290
2b (R = Ph) (folded)	−1434.686464	0.496813	0.524621	−1430.528961
2c (R = OCH_3) (folded)	−1201.705875	0.401152	0.424383	−1198.231814
2d (R = CHO) (folded)	−1199.315624	0.353803	0.376443	−1195.881669
Complex: **2a** (R = H) ··· Na^+ (4.4 Å)	−1134.857315	0.335822	0.356347	−1131.529874
Complex: **2b** (R = Ph) ··· Na^+ (8.7 Å)	−1596.806592	0.499353	0.528883	−1592.244261
Complex: **2c** (R = OCH_3) ··· Na^+ (4.3 Å)	−1363.824068	0.402030	0.426768	−1359.947407
Complex: **2c** (R = OCH_3) ··· Na^+ (7.3 Å)	−1363.823821	0.400518	0.426765	−1359.960517
Complex: **2d** (R = CHO) ··· Na^+ (8.9 Å)	−1361.452006	0.355158	0.379732	−1357.619386
Complex: **2d** (R = CHO) ··· Li^+ (8.3 Å)	−1206.721856	0.356609	0.380462	−1203.228298
Complex: **2d** (R = CHO) ··· NH_4^+ (9.8 Å)	−1256.253996	0.405067	0.431110	−1252.676357
Li^+	−7.281049	---	0.002360	−7.235485
Na^+	−162.044508	---	0.002360	−161.659283
NH_4^+	−56.866871	---	0.053730	−56.731035

[a] For the complexes is presented, in parenthesis, the distance between Fe of the ferrocene and the cation, *d*(Fe···cation).

Table S8. Electronic energies, E_{el}, and unscaled ZPE and T_cH (to 298.15 K), obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory for the systems studied, and MP2/6-31+G(d,p)/SDD(Fe) electronic energies, E_{el} (MP2), obtained from a single point energy calculation on the M06-2X/6-31+G(d,p)/SDD(Fe) optimized geometries, in CH_2Cl_2 and EtOH using the Polarizable Continuum Model (PCM) as a self-consistent reaction field. The optimized geometries were obtained in solution (PCM) using M06-2X/6-31+G(d,p)/SDD(Fe). Below are presented the solvation enthalpies, at T =298.15 K, for each species, calculated at the M06-2X/6-31+G(d,p)/SDD(Fe) level.

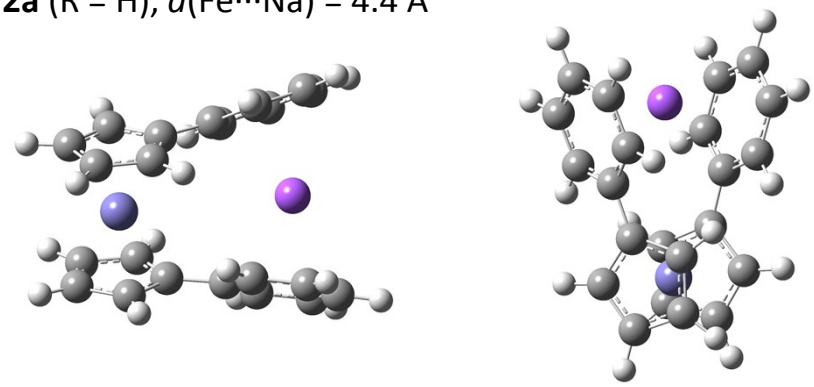
Molecular system [a]	E_{el} / hartree	ZPE / hartree	T_cH / hartree	E_{el} (MP2) / hartree
Na^+ in CH_2Cl_2	−162.187814	−−−	0.002360	−161.802551
Na^+ in EtOH	−162.199392	−−−	0.002360	−161.814126
2d (R = CHO) (folded) in CH_2Cl_2	−1199.329141	0.353672	0.376320	−1195.892664
2d (R = CHO) (folded) in EtOH	−1199.331155	0.353673	0.376316	−1195.894189
Complex: **2d** (R = CHO) ··· Na^+ (9.3 Å) in CH_2Cl_2	−1361.533493	0.354910	0.379452	−1357.698645
Complex: **2d** (R = CHO) ··· Na^+ (9.4 Å) in EtOH	−1361.541705	0.354489	0.379277	−1357.705672

Solvent	Molecular system	$\Delta_{solv}H_m$ / kJ·mol^{-1}
CH_2Cl_2	Na^+	−376
	2d (R = CHO) (folded)	−36
	Complex: **2d** (R = CHO) ··· Na^+	−211
EtOH	Na^+	−407
	2d (R = CHO) (folded)	−41
	Complex: **2d** (R = CHO) ··· Na^+	−234

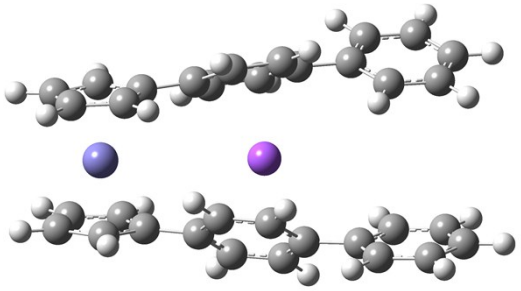
3.3. Optimized geometries.

Geometries obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

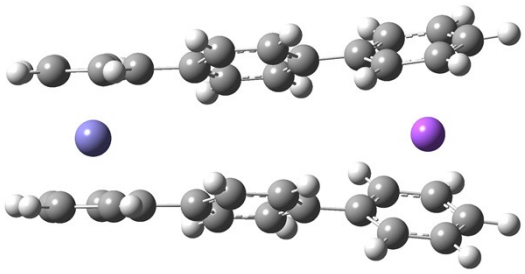
2a (R = H), *d*(Fe···Na) = 4.4 Å



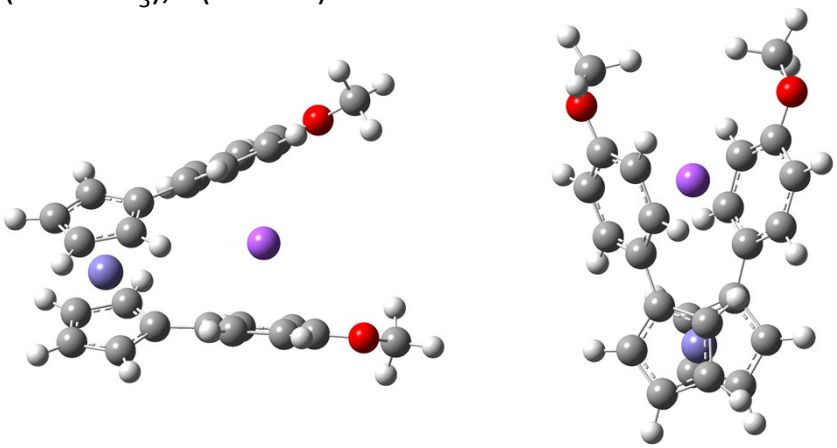
2b (R = Ph), *d*(Fe···Na) = 4.4 Å



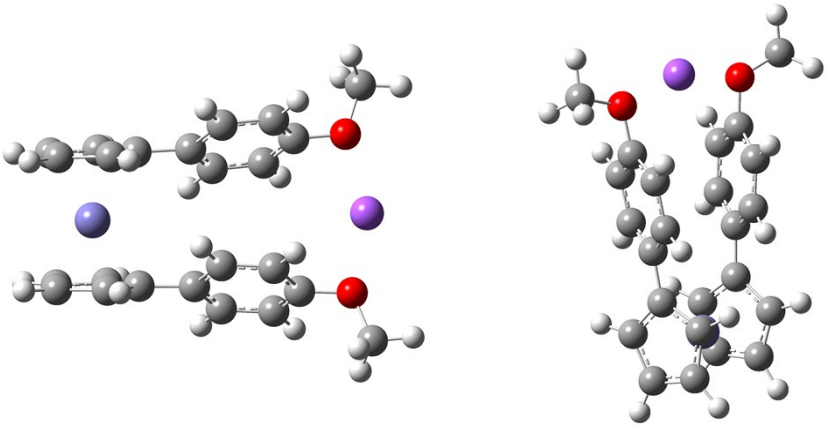
2b (R = Ph), *d*(Fe···Na) = 8.7 Å



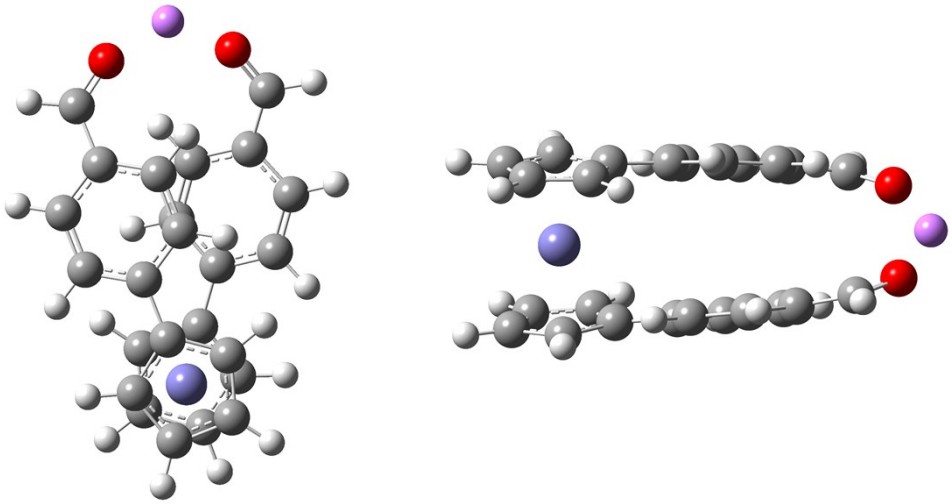
2c (R = OCH_3), *d*(Fe···Na) = 4.3 Å



2c (R = OCH_3), *d*(Fe···Na) = 7.3 Å



2d (R = CHO), *d*(Fe···Li) = 8.3 Å



2d (R = CHO), *d*(Fe···NH_4) = 9.8 Å

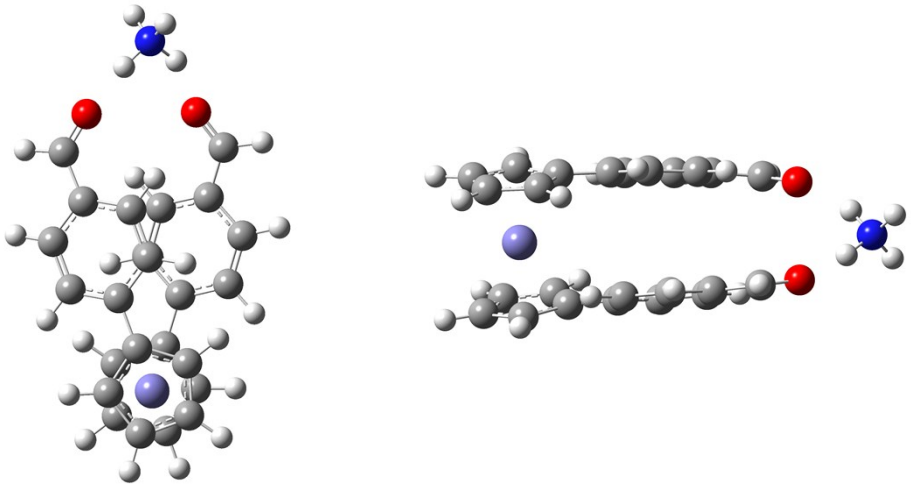


Table S9. Optimized geometries in Cartesian coordinates for the molecular systems considered, obtained at the M06-2X/6-31+G(d,p)/SDD(Fe) level of theory.

A) 1,1'-Diphenylferrocene

6	0	-2.927498	-1.717260	0.727048
6	0	-2.849763	-1.777427	-0.690453
6	0	-1.476888	-1.806193	-1.051773
6	0	-0.695773	-1.765910	0.140533
6	0	-1.603982	-1.705346	1.238301
1	0	-3.834607	-1.660284	1.312720
1	0	-3.687166	-1.761451	-1.374140
1	0	-1.084655	-1.805545	-2.060487
1	0	-1.324495	-1.657422	2.282226
26	0	-1.904997	-0.000001	-0.000001
6	0	-2.927502	1.717258	-0.727046
6	0	-2.849766	1.777422	0.690455
6	0	-1.603986	1.705348	-1.238301
1	0	-3.834612	1.660282	-1.312718
6	0	-1.476890	1.806189	1.051774
1	0	-3.687168	1.761442	1.374143
6	0	-0.695776	1.765911	-0.140533
1	0	-1.324501	1.657426	-2.282226
1	0	-1.084657	1.805539	2.060487
6	0	0.777536	-1.784671	0.222692
6	0	1.450212	-1.124030	1.259508
6	0	1.531425	-2.465512	-0.738943
6	0	2.838420	-1.141476	1.329392
1	0	0.878146	-0.559886	1.992168
6	0	2.923633	-2.481841	-0.671067
1	0	1.021288	-2.998730	-1.536449
6	0	3.581776	-1.821088	0.363751
1	0	3.343278	-0.605600	2.127433
1	0	3.492524	-3.017767	-1.425037
6	0	0.777532	1.784673	-0.222692
6	0	1.450209	1.124032	-1.259508
6	0	1.531421	2.465514	0.738943
6	0	2.838417	1.141479	-1.329393
1	0	0.878143	0.559888	-1.992169
6	0	2.923629	2.481843	0.671067
1	0	1.021284	2.998732	1.536449
6	0	3.581772	1.821090	-0.363751
1	0	3.343275	0.605604	-2.127433
1	0	3.492520	3.017770	1.425037
1	0	4.666196	-1.828438	0.415426
1	0	4.666192	1.828442	-0.415426

B) 1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene

6	0	4.990099	1.822565	0.406239
6	0	4.914599	1.625937	-0.998785
6	0	3.542431	1.585849	-1.361309
6	0	2.759035	1.758121	-0.182467
6	0	3.665860	1.899554	0.909463
1	0	5.896216	1.870972	0.994050
1	0	5.752229	1.489556	-1.668639
1	0	3.152131	1.405036	-2.354467
1	0	3.385543	2.039124	1.944844

26	0	3.971030	-0.000144	-0.000067
6	0	4.989743	-1.823089	-0.406288
6	0	4.914348	-1.626334	0.998722
6	0	3.665464	-1.899869	-0.909442
1	0	5.895827	-1.871700	-0.994132
6	0	3.542204	-1.585946	1.361312
1	0	5.752039	-1.490026	1.668517
6	0	2.758724	-1.758184	0.182522
1	0	3.385063	-2.039503	-1.944792
1	0	3.151982	-1.404966	2.354470
6	0	1.286663	1.777501	-0.103700
6	0	0.619410	1.334479	1.045593
6	0	0.518035	2.236870	-1.178067
6	0	-0.766855	1.348973	1.116148
1	0	1.194745	0.930969	1.875506
6	0	-0.872030	2.245591	-1.109510
1	0	1.014255	2.614020	-2.068076
6	0	-1.538637	1.803076	0.038414
1	0	-1.261543	0.961710	2.003410
1	0	-1.448617	2.630249	-1.946549
6	0	1.286339	-1.777294	0.103805
6	0	0.619115	-1.334106	-1.045437
6	0	0.517684	-2.236663	1.178156
6	0	-0.767153	-1.348490	-1.115976
1	0	1.194472	-0.930555	-1.875315
6	0	-0.872383	-2.245343	1.109594
1	0	1.013893	-2.613888	2.068140
6	0	-1.538951	-1.802742	-0.038324
1	0	-1.261854	-0.961123	-2.003189
1	0	-1.448997	-2.630023	1.946604
6	0	-3.019815	1.816946	0.113285
6	0	-3.672168	2.221022	1.284394
6	0	-3.796742	1.428084	-0.986077
6	0	-5.063621	2.244532	1.352572
1	0	-3.082842	2.544152	2.138280
6	0	-5.186046	1.453375	-0.919925
1	0	-3.305062	1.072709	-1.888092
6	0	-5.825191	1.865081	0.249112
1	0	-5.552528	2.571252	2.265674
1	0	-5.770898	1.131205	-1.776134
1	0	-6.909592	1.881417	0.301466
6	0	-3.020116	-1.816734	-0.113254
6	0	-3.672337	-2.220932	-1.284390
6	0	-3.797150	-1.427875	0.986029
6	0	-5.063789	-2.244642	-1.352651
1	0	-3.082925	-2.544016	-2.138233
6	0	-5.186443	-1.453369	0.919791
1	0	-3.305562	-1.072356	1.888038
6	0	-5.825477	-1.865265	-0.249247
1	0	-5.552587	-2.571472	-2.265773
1	0	-5.771379	-1.131249	1.775961
1	0	-6.909873	-1.881823	-0.301636

C) 1,1'-Bis(4-methoxyphenyl)ferrocene

6	0	-3.797268	1.776090	-0.511422
6	0	-3.630082	1.716136	0.897837
6	0	-2.236609	1.712891	1.171627
6	0	-1.531491	1.774600	-0.065700
6	0	-2.507862	1.807943	-1.104621

1	0	-4.739433	1.766988	-1.041785
1	0	-4.421700	1.641586	1.630536
1	0	-1.781522	1.626213	2.149850
1	0	-2.295833	1.845736	-2.164757
26	0	-2.742715	-0.000011	0.000006
6	0	-3.797232	-1.776141	0.511441
6	0	-3.630052	-1.716188	-0.897818
6	0	-2.507821	-1.807961	1.104638
1	0	-4.739397	-1.767068	1.041803
6	0	-2.236580	-1.712906	-1.171614
1	0	-4.421671	-1.641662	-1.630518
6	0	-1.531459	-1.774606	0.065711
1	0	-2.295780	-1.845745	2.164771
1	0	-1.781498	-1.626205	-2.149838
6	0	-0.066279	1.757529	-0.236983
6	0	0.517267	1.133332	-1.350765
6	0	0.782400	2.322610	0.713946
6	0	1.890481	1.056823	-1.491876
1	0	-0.122176	0.661824	-2.093172
6	0	2.172397	2.240993	0.595061
1	0	0.355189	2.832550	1.573355
6	0	2.728189	1.588014	-0.504569
1	0	2.343887	0.546262	-2.335599
1	0	2.799052	2.672039	1.367053
6	0	-0.066241	-1.757493	0.236965
6	0	0.517326	-1.133354	1.350761
6	0	0.782423	-2.322516	-0.714015
6	0	1.890546	-1.056879	1.491871
1	0	-0.122100	-0.661912	2.093223
6	0	2.172420	-2.240924	-0.595141
1	0	0.355188	-2.832399	-1.573446
6	0	2.728247	-1.588033	0.504541
1	0	2.343952	-0.546394	2.335641
1	0	2.799057	-2.671968	-1.367143
8	0	4.063143	1.401626	-0.702443
8	0	4.063215	-1.401679	0.702462
6	0	4.929421	1.719617	0.367530
1	0	4.659849	1.148324	1.264141
1	0	5.929962	1.434281	0.040903
1	0	4.916912	2.794097	0.586074
6	0	4.929602	-1.719511	-0.367480
1	0	4.659980	-1.148273	-1.264105
1	0	5.930073	-1.433977	-0.040815
1	0	4.917286	-2.793994	-0.586030

D) 4,4’-(Ferrocen-1,1’-diyl)dibenzaldehyde

6	0	-3.678102	1.682619	-0.812199
6	0	-3.613325	1.805997	0.602045
6	0	-2.245620	1.854763	0.974895
6	0	-1.453161	1.761420	-0.207933
6	0	-2.351601	1.649576	-1.311149
1	0	-4.580031	1.599482	-1.402572
1	0	-4.456979	1.820280	1.277905
1	0	-1.865314	1.902285	1.986752
1	0	-2.065779	1.557459	-2.350258
26	0	-2.656633	-0.000002	0.000002
6	0	-3.678089	-1.682630	0.812204
6	0	-3.613316	-1.806006	-0.602041
6	0	-2.351586	-1.649583	1.311148

1	0	-4.580017	-1.599498	1.402580
6	0	-2.245613	-1.854760	-0.974896
1	0	-4.456972	-1.820292	-1.277899
6	0	-1.453150	-1.761418	0.207929
1	0	-2.065761	-1.557467	2.350257
1	0	-1.865309	-1.902276	-1.986755
6	0	0.018891	1.764109	-0.273396
6	0	0.692246	1.109457	-1.313973
6	0	0.770622	2.416415	0.716913
6	0	2.080251	1.095812	-1.355595
1	0	0.121606	0.573825	-2.067843
6	0	2.157565	2.390936	0.685489
1	0	0.255820	2.949972	1.510443
6	0	2.819366	1.725317	-0.351127
1	0	2.598322	0.564400	-2.151302
1	0	2.749046	2.880974	1.453525
6	0	0.018903	-1.764100	0.273388
6	0	0.692257	-1.109523	1.314013
6	0	0.770633	-2.416346	-0.716961
6	0	2.080261	-1.095890	1.355641
1	0	0.121616	-0.573959	2.067930
6	0	2.157577	-2.390861	-0.685539
1	0	0.255830	-2.949848	-1.510528
6	0	2.819376	-1.725320	0.351127
1	0	2.598333	-0.564545	2.151393
1	0	2.749059	-2.880850	-1.453605
6	0	4.297360	1.642945	-0.366581
8	0	5.009409	2.072926	0.515355
1	0	4.736818	1.132992	-1.248319
6	0	4.297371	-1.642955	0.366594
8	0	5.009425	-2.072892	-0.515361
1	0	4.736823	-1.133000	1.248333

E) 1,1'-Diphenylferrocene···Na^+ (4.4 Å) complex

6	0	3.123419	-1.760579	0.302923
6	0	2.725116	-1.238998	1.562829
6	0	1.309371	-1.245676	1.613681
6	0	0.822163	-1.767170	0.377344
6	0	1.956122	-2.082379	-0.431635
1	0	4.140303	-1.866898	-0.048105
1	0	3.385965	-0.868571	2.333955
1	0	0.702738	-0.887556	2.435779
1	0	1.926600	-2.503786	-1.427577
26	0	1.956121	-0.000216	0.000060
6	0	3.124011	1.759863	-0.302883
6	0	2.725464	1.238801	-1.562807
6	0	1.956700	2.082008	0.431518
1	0	4.140885	1.866297	0.048096
6	0	1.309749	1.245824	-1.613645
1	0	3.385944	0.868288	-2.334212
6	0	0.822553	1.766972	-0.377287
1	0	1.927142	2.503127	1.427582
1	0	0.703165	0.887683	-2.435792
6	0	-0.586913	-1.988522	0.011137
6	0	-1.014315	-1.896421	-1.326531
6	0	-1.533321	-2.343810	0.988978
6	0	-2.339421	-2.163520	-1.677020
1	0	-0.295837	-1.619528	-2.093460
6	0	-2.862851	-2.602460	0.640385

1	0	-1.213679	-2.457616	2.020620
6	0	-3.272863	-2.514760	-0.694113
1	0	-2.642609	-2.107965	-2.717991
1	0	-3.570737	-2.900850	1.407678
6	0	-0.586410	1.988726	-0.010930
6	0	-1.013958	1.895660	1.326609
6	0	-1.532568	2.345164	-0.988635
6	0	-2.339089	2.162740	1.677116
1	0	-0.295645	1.618061	2.093451
6	0	-2.862081	2.603881	-0.640022
1	0	-1.212667	2.459723	-2.020121
6	0	-3.272288	2.515049	0.694371
1	0	-2.642462	2.106347	2.718002
1	0	-3.569814	2.903157	-1.407119
1	0	-4.298002	-2.741836	-0.967832
1	0	-4.297444	2.742029	0.968149
11	0	-2.462229	0.000287	-0.000997

F) 1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene···Na^+ (8.7 Å) complex

6	0	5.067338	-1.443710	-1.270028
6	0	5.194840	-1.851412	0.084726
6	0	3.892826	-2.019672	0.616831
6	0	2.944879	-1.717530	-0.408424
6	0	3.686868	-1.358195	-1.575460
1	0	5.880442	-1.210914	-1.943212
1	0	6.122123	-1.975441	0.626342
1	0	3.665253	-2.287647	1.639669
1	0	3.272769	-1.065683	-2.530574
26	0	4.141079	0.000577	-0.002316
6	0	5.069481	1.447213	1.260201
6	0	5.188702	1.855238	-0.095374
6	0	3.690755	1.357644	1.573145
1	0	5.886958	1.216908	1.928937
6	0	3.883280	2.020683	-0.620217
1	0	6.112810	1.980823	-0.642065
6	0	2.942140	1.715915	0.410135
1	0	3.280869	1.066769	2.530684
1	0	3.647033	2.285548	-1.642039
6	0	1.479263	-1.768819	-0.283700
6	0	0.641517	-1.186021	-1.246911
6	0	0.878772	-2.429153	0.796320
6	0	-0.739008	-1.287051	-1.148599
1	0	1.076124	-0.635480	-2.075800
6	0	-0.503205	-2.510263	0.909644
1	0	1.499189	-2.916180	1.541563
6	0	-1.334170	-1.951525	-0.067781
1	0	-1.360485	-0.816283	-1.907813
1	0	-0.937823	-3.063027	1.738175
6	0	1.476237	1.768326	0.292784
6	0	0.640676	1.129133	1.221132
6	0	0.873059	2.489813	-0.745538
6	0	-0.740218	1.225649	1.125308
1	0	1.078132	0.530389	2.014617
6	0	-0.508947	2.575290	-0.851090
1	0	1.492411	3.024616	-1.458282
6	0	-1.340327	1.952473	0.087261
1	0	-1.357008	0.699253	1.850430
1	0	-0.940639	3.183056	-1.641276
6	0	-2.803136	-2.099221	0.037195

6	0	-3.585995	-2.383098	-1.098341
6	0	-3.454347	-2.000739	1.281762
6	0	-4.966064	-2.575674	-0.990313
1	0	-3.099249	-2.501352	-2.062069
6	0	-4.833174	-2.198943	1.392257
1	0	-2.871133	-1.769915	2.168907
6	0	-5.597296	-2.487014	0.256035
1	0	-5.544369	-2.825835	-1.874388
1	0	-5.309366	-2.134756	2.365926
1	0	-6.664655	-2.661805	0.343331
6	0	-2.810513	2.099102	-0.008523
6	0	-3.612900	2.176487	1.146638
6	0	-3.449073	2.205405	-1.259984
6	0	-4.993808	2.367734	1.054764
1	0	-3.142607	2.132397	2.124395
6	0	-4.828462	2.409102	-1.353598
1	0	-2.856699	2.135611	-2.167686
6	0	-5.610430	2.489408	-0.195863
1	0	-5.584995	2.450572	1.961633
1	0	-5.291111	2.513350	-2.330385
1	0	-6.678613	2.666677	-0.266009
11	0	-4.552798	-0.012373	-0.199196

G) 1,1'-Bis(4-methoxyphenyl)ferrocene···Na^+ (4.3 Å) complex

6	0	3.867366	-1.736680	0.439331
6	0	3.469661	-1.119425	1.654520
6	0	2.052799	-1.117628	1.702934
6	0	1.565290	-1.735222	0.512340
6	0	2.698996	-2.114223	-0.267423
1	0	4.883990	-1.869541	0.096885
1	0	4.130536	-0.692924	2.396190
1	0	1.447030	-0.692243	2.493253
1	0	2.670441	-2.610894	-1.228128
26	0	2.706548	-0.001198	0.003474
6	0	3.876321	1.728428	-0.426989
6	0	3.478729	1.115855	-1.644579
6	0	2.707635	2.109619	0.278190
1	0	4.892686	1.855799	-0.081692
6	0	2.061814	1.121245	-1.696718
1	0	4.139582	0.687708	-2.385338
6	0	1.574694	1.737812	-0.505792
1	0	2.676795	2.603111	1.240555
1	0	1.454285	0.699971	-2.488047
6	0	0.155130	-1.989281	0.167135
6	0	-0.274668	-2.047771	-1.175414
6	0	-0.800361	-2.234726	1.161451
6	0	-1.591665	-2.345850	-1.504128
1	0	0.442157	-1.858627	-1.970123
6	0	-2.136466	-2.525458	0.849540
1	0	-0.495960	-2.231898	2.204103
6	0	-2.536984	-2.603463	-0.491860
1	0	-1.913979	-2.413295	-2.538360
1	0	-2.833990	-2.731314	1.653094
6	0	0.164245	1.992813	-0.161587
6	0	-0.282800	1.966089	1.175929
6	0	-0.773079	2.316997	-1.150222
6	0	-1.601025	2.255763	1.506437
1	0	0.422063	1.712377	1.963330
6	0	-2.110401	2.602008	-0.837056

1	0	-0.451911	2.380471	-2.186038
6	0	-2.528793	2.592307	0.501232
1	0	-1.937971	2.255035	2.538237
1	0	-2.793589	2.872401	-1.633788
8	0	-3.783565	-2.898183	-0.907434
8	0	-3.778057	2.871435	0.919197
6	0	-4.747860	-3.277485	0.066549
1	0	-4.959726	-2.450051	0.753406
1	0	-5.648547	-3.527434	-0.490268
1	0	-4.407857	-4.152756	0.629360
6	0	-4.726275	3.320950	-0.040888
1	0	-4.930053	2.543441	-0.785902
1	0	-5.634526	3.536781	0.517988
1	0	-4.373957	4.231006	-0.537119
11	0	-1.638963	0.001996	-0.093058

H) 1,1'-Bis(4-methoxyphenyl)ferrocene···Na^+ (7.3 Å) complex

6	0	-3.968203	1.827595	-0.344168
6	0	-3.863332	1.600635	1.054183
6	0	-2.486488	1.557125	1.390884
6	0	-1.729422	1.751741	0.197689
6	0	-2.657351	1.917417	-0.874822
1	0	-4.886767	1.890701	-0.910521
1	0	-4.687238	1.449693	1.737557
1	0	-2.080733	1.362727	2.375476
1	0	-2.400737	2.087703	-1.911925
26	0	-2.925762	0.000774	-0.000772
6	0	-3.969806	-1.824772	0.344503
6	0	-3.864691	-1.599744	-1.054127
6	0	-2.659062	-1.914968	0.875357
1	0	-4.888425	-1.886275	0.910947
6	0	-2.487798	-1.557829	-1.390805
1	0	-4.688387	-1.448994	-1.737792
6	0	-1.730951	-1.751461	-0.197289
1	0	-2.402740	-2.083773	1.912776
1	0	-2.081708	-1.365261	-2.375614
6	0	-0.261947	1.806965	0.083285
6	0	0.386173	1.371175	-1.080503
6	0	0.513978	2.329688	1.126440
6	0	1.765422	1.488427	-1.217675
1	0	-0.197202	0.931414	-1.885136
6	0	1.897481	2.435370	1.010406
1	0	0.025277	2.683492	2.029208
6	0	2.508771	2.028201	-0.171022
1	0	2.263919	1.178964	-2.133283
1	0	2.496246	2.853425	1.814790
6	0	-0.263505	-1.807423	-0.082907
6	0	0.384914	-1.370023	1.080256
6	0	0.512005	-2.332105	-1.125251
6	0	1.764067	-1.486963	1.217455
1	0	-0.198312	-0.928535	1.884044
6	0	1.895551	-2.438360	-1.008912
1	0	0.023131	-2.687352	-2.027348
6	0	2.507024	-2.029138	0.171685
1	0	2.263173	-1.174758	2.131739
1	0	2.494117	-2.858988	-1.812127
8	0	3.898621	2.116884	-0.305456
8	0	3.896958	-2.118600	0.305615
6	0	4.365560	3.427243	-0.666713

1	0	4.085913	4.147921	0.106072
1	0	5.450727	3.367899	-0.746537
1	0	3.930899	3.720858	-1.626218
6	0	4.361257	-3.424132	0.687255
1	0	4.076153	-4.156399	-0.072423
1	0	5.446850	-3.367175	0.762387
1	0	3.929072	-3.700263	1.652980
11	0	4.383097	-0.004672	-0.019224

I) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde···Li^+ (8.3 Å) complex

6	0	3.761013	1.469348	-1.088009
6	0	3.302008	0.466022	-1.985186
6	0	1.888991	0.447895	-1.939450
6	0	1.456256	1.441839	-1.004273
6	0	2.632835	2.070333	-0.484051
1	0	4.793704	1.715143	-0.883769
1	0	3.925196	-0.190724	-2.576001
1	0	1.252603	-0.241835	-2.478557
1	0	2.666381	2.862252	0.251366
26	0	2.630728	-0.000010	0.000013
6	0	3.760962	-1.469412	1.088027
6	0	3.301968	-0.466092	1.985216
6	0	2.632778	-2.070360	0.484043
1	0	4.793650	-1.715227	0.883798
6	0	1.888951	-0.447933	1.939464
1	0	3.925163	0.190628	2.576053
6	0	1.456207	-1.441848	1.004261
1	0	2.666314	-2.862266	-0.251389
1	0	1.252572	0.241802	2.478573
6	0	0.073859	1.687716	-0.577497
6	0	-0.195138	2.432247	0.585126
6	0	-1.011005	1.169717	-1.313599
6	0	-1.497237	2.634483	1.010223
1	0	0.626436	2.845828	1.160443
6	0	-2.309747	1.339193	-0.873107
1	0	-0.822806	0.629517	-2.235427
6	0	-2.567321	2.065130	0.302265
1	0	-1.692475	3.213876	1.909513
1	0	-3.139434	0.924309	-1.439050
6	0	0.073807	-1.687699	0.577476
6	0	-0.195195	-2.432175	-0.585182
6	0	-1.011054	-1.169732	1.313604
6	0	-1.497295	-2.634392	-1.010283
1	0	0.626378	-2.845725	-1.160524
6	0	-2.309799	-1.339198	0.873116
1	0	-0.822849	-0.629570	2.235454
6	0	-2.567377	-2.065085	-0.302285
1	0	-1.692537	-3.213746	-1.909597
1	0	-3.139485	-0.924348	1.439086
6	0	-3.903710	2.195040	0.846575
8	0	-4.883490	1.543852	0.475441
1	0	-4.035995	2.915395	1.669947
6	0	-3.903774	-2.194999	-0.846579
8	0	-4.883568	-1.543862	-0.475389
1	0	-4.036046	-2.915291	-1.670008
3	0	-5.658375	0.000031	-0.000016

J) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde···Na^+ (8.9 Å) complex

6	0	-4.007950	1.485591	1.067142
6	0	-3.553700	0.492692	1.977730
6	0	-2.139907	0.469343	1.933626
6	0	-1.702942	1.448501	0.986001
6	0	-2.876157	2.074563	0.456812
1	0	-5.039474	1.732499	0.858408
1	0	-4.179724	-0.154535	2.576000
1	0	-1.505515	-0.215852	2.480841
1	0	-2.904458	2.857402	-0.288576
26	0	-2.882562	-0.001577	-0.000042
6	0	-4.004286	-1.488989	-1.070208
6	0	-3.550423	-0.493936	-1.978672
6	0	-2.872339	-2.077153	-0.459301
1	0	-5.035701	-1.737713	-0.863103
6	0	-2.136694	-0.468535	-1.932814
1	0	-4.176667	0.153486	-2.576503
6	0	-1.699460	-1.448503	-0.986154
1	0	-2.900175	-2.861501	0.284526
1	0	-1.502591	0.218864	-2.477630
6	0	-0.318065	1.685011	0.556854
6	0	-0.047646	2.386282	-0.630851
6	0	0.765104	1.197699	1.314467
6	0	1.256536	2.581371	-1.055762
1	0	-0.869137	2.769168	-1.227449
6	0	2.066771	1.366710	0.878899
1	0	0.574178	0.681733	2.249693
6	0	2.325470	2.055505	-0.316570
1	0	1.452811	3.126722	-1.976001
1	0	2.899103	0.973920	1.456146
6	0	-0.314682	-1.683996	-0.556112
6	0	-0.044592	-2.382997	0.632985
6	0	0.768617	-1.198324	-1.314551
6	0	1.259531	-2.577977	1.058150
1	0	-0.866343	-2.764065	1.230418
6	0	2.070236	-1.366924	-0.878581
1	0	0.577794	-0.684125	-2.250791
6	0	2.328667	-2.053865	0.317997
1	0	1.455592	-3.121778	1.979351
1	0	2.902691	-0.975453	-1.456551
6	0	3.673421	2.193105	-0.844616
8	0	4.665492	1.622946	-0.396237
1	0	3.785358	2.845512	-1.728267
6	0	3.676633	-2.191558	0.846177
8	0	4.669018	-1.622457	0.397235
1	0	3.788229	-2.843113	1.730499
11	0	6.025612	0.001292	-0.002162

K) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde···NH_4^+ (9.8 Å) complex

6	0	4.077000	-1.706022	0.681201
6	0	3.702740	-0.907994	1.796749
6	0	2.289791	-0.836522	1.831750
6	0	1.773440	-1.590127	0.730106
6	0	2.896620	-2.125945	0.024020
1	0	5.087722	-1.932733	0.372399
1	0	4.379235	-0.412949	2.479259
1	0	1.708135	-0.263478	2.541405
1	0	2.860309	-2.739120	-0.865651

26	0	2.966519	-0.000013	0.000001
6	0	4.077042	1.705978	-0.681181
6	0	3.702777	0.907962	-1.796737
6	0	2.896664	2.125923	-0.024012
1	0	5.087767	1.932666	-0.372369
6	0	2.289827	0.836518	-1.831753
1	0	4.379270	0.412910	-2.479243
6	0	1.773480	1.590130	-0.730112
1	0	2.860353	2.739086	0.865667
1	0	1.708168	0.263502	-2.541427
6	0	0.360179	-1.717025	0.350072
6	0	-0.005510	-2.188665	-0.922327
6	0	-0.658013	-1.360186	1.256266
6	0	-1.340831	-2.295488	-1.279733
1	0	0.764171	-2.464152	-1.635666
6	0	-1.990101	-1.452399	0.898543
1	0	-0.392323	-1.016393	2.250116
6	0	-2.344280	-1.919865	-0.376549
1	0	-1.611483	-2.662135	-2.267176
1	0	-2.775104	-1.173075	1.595072
6	0	0.360219	1.717038	-0.350078
6	0	-0.005470	2.188708	0.922309
6	0	-0.657973	1.360175	-1.256263
6	0	-1.340791	2.295535	1.279714
1	0	0.764210	2.464217	1.635641
6	0	-1.990060	1.452393	-0.898541
1	0	-0.392285	1.016358	-2.250105
6	0	-2.344239	1.919886	0.376542
1	0	-1.611442	2.662205	2.267149
1	0	-2.775063	1.173050	-1.595062
6	0	-3.736879	-1.979752	-0.792565
8	0	-4.681200	-1.609838	-0.099122
1	0	-3.925765	-2.374682	-1.807057
6	0	-3.736838	1.979776	0.792558
8	0	-4.681155	1.609821	0.099131
1	0	-3.925726	2.374744	1.807035
1	0	-6.159263	0.812368	0.167802
7	0	-6.802124	0.000023	0.000003
1	0	-7.390080	-0.176487	0.814126
1	0	-7.390082	0.176534	-0.814118
1	0	-6.159265	-0.812325	-0.167797

L) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde PCM (CH_2Cl_2)

6	0	3.679139	1.691993	0.790325
6	0	3.613043	1.798125	-0.626411
6	0	2.245127	1.841675	-1.000029
6	0	1.454007	1.760792	0.185686
6	0	2.353138	1.663184	1.291511
1	0	4.581667	1.613179	1.380765
1	0	4.456378	1.801084	-1.303163
1	0	1.864737	1.874029	-2.012639
1	0	2.069431	1.577865	2.332040
26	0	2.655518	-0.000004	-0.000001
6	0	3.679120	-1.692011	-0.790331
6	0	3.613030	-1.798141	0.626406
6	0	2.353116	-1.663194	-1.291511
1	0	4.581646	-1.613205	-1.380775
6	0	2.245115	-1.841674	1.000030
1	0	4.456368	-1.801108	1.303153

6	0	1.453991	-1.760791	-0.185681
1	0	2.069405	-1.577875	-2.332039
1	0	1.864727	-1.874021	2.012642
6	0	-0.017410	1.760661	0.253706
6	0	-0.685196	1.124695	1.310461
6	0	-0.773810	2.393089	-0.747414
6	0	-2.072534	1.113558	1.360107
1	0	-0.112001	0.604693	2.073031
6	0	-2.160369	2.374146	-0.705008
1	0	-0.264735	2.904866	-1.558510
6	0	-2.817501	1.731501	0.350575
1	0	-2.585505	0.601216	2.171100
1	0	-2.748623	2.853841	-1.481695
6	0	-0.017427	-1.760648	-0.253697
6	0	-0.685212	-1.124774	-1.310509
6	0	-0.773829	-2.392997	0.747471
6	0	-2.072549	-1.113650	-1.360164
1	0	-0.112015	-0.604850	-2.073132
6	0	-2.160388	-2.374044	0.705070
1	0	-0.264753	-2.904708	1.558608
6	0	-2.817517	-1.731494	-0.350572
1	0	-2.585521	-0.601390	-2.171209
1	0	-2.748643	-2.853672	1.481798
6	0	-4.289922	1.667107	0.401777
8	0	-5.029788	2.127123	-0.448327
1	0	-4.710308	1.147612	1.285244
6	0	-4.289937	-1.667101	-0.401782
8	0	-5.029807	-2.127091	0.448334
1	0	-4.710323	-1.147737	-1.285326

M) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde PCM (EtOH)

6	0	-3.679439	1.694696	-0.784493
6	0	-3.612868	1.796224	0.632757
6	0	-2.244830	1.838136	1.006393
6	0	-1.454136	1.760627	-0.180007
6	0	-2.353594	1.666934	-1.286219
1	0	-4.582164	1.617450	-1.374895
1	0	-4.456024	1.796554	1.309788
1	0	-1.864257	1.866315	2.019078
1	0	-2.070278	1.583728	-2.327048
26	0	-2.655768	-0.000097	0.000029
6	0	-3.679200	-1.695012	0.784598
6	0	-3.612685	-1.796530	-0.632656
6	0	-2.353335	-1.667093	1.286262
1	0	-4.581908	-1.617874	1.375042
6	0	-2.244659	-1.838279	-1.006356
1	0	-4.455872	-1.796960	-1.309648
6	0	-1.453918	-1.760678	0.180007
1	0	-2.069981	-1.583854	2.327077
1	0	-1.864130	-1.866411	-2.019059
6	0	0.017148	1.759056	-0.249325
6	0	0.682419	1.128552	-1.311090
6	0	0.775857	2.384358	0.754798
6	0	2.069584	1.116657	-1.363322
1	0	0.107786	0.613694	-2.076047
6	0	2.162282	2.365022	0.709423
1	0	0.269006	2.889953	1.571095
6	0	2.817026	1.728805	-0.351796
1	0	2.580383	0.608959	-2.178526

1	0	2.751391	2.839233	1.488822
6	0	0.017368	-1.758930	0.249255
6	0	0.682614	-1.128351	1.310991
6	0	0.776104	-2.384134	-0.754908
6	0	2.069780	-1.116291	1.363158
1	0	0.107956	-0.613565	2.075978
6	0	2.162528	-2.364629	-0.709601
1	0	0.269274	-2.889784	-1.571186
6	0	2.817247	-1.728327	0.351582
1	0	2.580557	-0.608532	2.178338
1	0	2.751657	-2.838754	-1.489038
6	0	4.288411	1.664646	-0.409423
8	0	5.033457	2.122301	0.438459
1	0	4.704449	1.146620	-1.295558
6	0	4.288626	-1.663925	0.409098
8	0	5.033725	-2.123053	-0.437939
1	0	4.704692	-1.147435	1.296116

N) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde···Na^+ complex PCM (CH_2Cl_2)

6	0	-4.058995	1.750801	0.565816
6	0	-3.719387	1.006569	1.728946
6	0	-2.306803	0.919577	1.798197
6	0	-1.757188	1.611269	0.672907
6	0	-2.857184	2.123257	-0.084649
1	0	-5.059680	1.966724	0.217822
1	0	-4.416430	0.551727	2.419285
1	0	-1.749143	0.374032	2.547859
1	0	-2.792691	2.679352	-1.009838
26	0	-2.962856	0.002033	0.000118
6	0	-4.065901	-1.742869	-0.564467
6	0	-3.724692	-1.000003	-1.727991
6	0	-2.864858	-2.119632	0.084925
1	0	-5.067039	-1.955120	-0.215527
6	0	-2.311892	-0.918091	-1.798554
1	0	-4.420729	-0.542780	-2.417772
6	0	-1.763735	-1.611558	-0.673610
1	0	-2.801620	-2.675818	1.010138
1	0	-1.753074	-0.374656	-2.548875
6	0	-0.330785	1.713095	0.320848
6	0	0.064830	2.177177	-0.943458
6	0	0.662262	1.346509	1.248401
6	0	1.410298	2.272102	-1.271844
1	0	-0.684652	2.455691	-1.677122
6	0	2.004320	1.424379	0.917605
1	0	0.374620	0.996793	2.234303
6	0	2.388448	1.888758	-0.347845
1	0	1.706901	2.629415	-2.254944
1	0	2.770163	1.126597	1.628384
6	0	-0.337498	-1.716382	-0.321795
6	0	0.057477	-2.182510	0.941948
6	0	0.656004	-1.349149	-1.248602
6	0	1.402810	-2.277914	1.270878
1	0	-0.692319	-2.461745	1.675006
6	0	1.997837	-1.427569	-0.917294
1	0	0.368890	-0.997972	-2.234133
6	0	2.381326	-1.893071	0.347931
1	0	1.698932	-2.636240	2.253754
1	0	2.764006	-1.128677	-1.627226
6	0	3.797330	1.926123	-0.743866

8	0	4.720332	1.524727	-0.048156
1	0	4.003938	2.334349	-1.749526
6	0	3.789889	-1.927767	0.745141
8	0	4.711904	-1.521284	0.051102
1	0	3.997097	-2.337880	1.749883
11	0	6.385977	-0.003892	-0.002319

O) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde···Na^+ complex PCM (EtOH)

6	0	-4.062823	1.753711	0.550724
6	0	-3.725559	1.017569	1.719847
6	0	-2.312797	0.931232	1.792612
6	0	-1.760944	1.615203	0.663733
6	0	-2.859282	2.121704	-0.099851
1	0	-5.062793	1.966304	0.198508
1	0	-4.423865	0.566698	2.411599
1	0	-1.756586	0.389877	2.546449
1	0	-2.792342	2.669839	-1.029659
26	0	-2.966301	0.001244	-0.000155
6	0	-4.066987	-1.748682	-0.551303
6	0	-3.728188	-1.013048	-1.720289
6	0	-2.864229	-2.119597	0.099042
1	0	-5.067396	-1.959059	-0.199003
6	0	-2.315263	-0.929865	-1.793188
1	0	-4.425555	-0.560444	-2.411858
6	0	-1.764823	-1.615302	-0.664473
1	0	-2.798551	-2.668100	1.028717
1	0	-1.758033	-0.389714	-2.547126
6	0	-0.333301	1.714521	0.313909
6	0	0.065089	2.164311	-0.954539
6	0	0.657257	1.357466	1.247547
6	0	1.411607	2.252238	-1.282139
1	0	-0.682611	2.434281	-1.693269
6	0	2.000254	1.429926	0.918106
1	0	0.367726	1.017381	2.236319
6	0	2.387203	1.878130	-0.352087
1	0	1.710407	2.595243	-2.269618
1	0	2.764120	1.137088	1.633111
6	0	-0.337460	-1.716581	-0.314141
6	0	0.059950	-2.169743	0.953409
6	0	0.653801	-1.357092	-1.246100
6	0	1.406216	-2.258132	1.281956
1	0	-0.688233	-2.441910	1.690829
6	0	1.996483	-1.429928	-0.915659
1	0	0.365081	-1.014490	-2.234234
6	0	2.382441	-1.880940	0.353836
1	0	1.704298	-2.603566	2.268805
1	0	2.760838	-1.134848	-1.629206
6	0	3.798600	1.903876	-0.746070
8	0	4.717112	1.518172	-0.036957
1	0	4.008542	2.286467	-1.760986
6	0	3.793372	-1.905658	0.749301
8	0	4.711571	-1.513758	0.043235
1	0	4.003295	-2.293125	1.762335
11	0	6.416575	-0.003408	-0.006637

P) Ferrocene

6	0	-1.759608	1.188518	-0.212051
6	0	-1.754035	0.165173	-1.197514
6	0	-1.751303	-1.088409	-0.529186
6	0	-1.754258	-0.840283	0.869692
6	0	-1.759143	0.567343	1.065838
1	0	-1.730867	2.252789	-0.400628
1	0	-1.718783	0.314946	-2.267856
1	0	-1.715244	-2.060090	-1.002078
1	0	-1.731567	1.076879	2.019050
26	0	0.000137	0.002279	0.001361
6	0	1.753122	-0.493800	-1.103574
6	0	1.755188	0.896532	-0.810865
6	0	1.754435	-1.201944	0.128066
6	0	1.757756	1.047681	0.602120
1	0	1.723871	1.698675	-1.535228
6	0	1.757525	-0.249489	1.182206
1	0	1.723284	-2.276517	0.243909
1	0	1.727839	1.984368	1.141199
1	0	1.723858	-0.472488	2.239718
1	0	1.720166	-0.935665	-2.089893
1	0	-1.724207	-1.590089	1.648029

Q) 1-Phenylferrocene

6	0	-1.711290	-1.846326	-0.740644
6	0	-1.008432	-1.928485	0.491663
6	0	-1.812651	-1.325026	1.495426
6	0	-3.011460	-0.868156	0.883766
6	0	-2.948975	-1.189932	-0.498753
1	0	-1.352831	-2.191313	-1.701035
1	0	-0.014217	-2.332041	0.630721
1	0	-1.541774	-1.199390	2.534556
1	0	-3.696498	-0.948715	-1.241869
26	0	-1.338684	0.111802	0.000550
6	0	0.533234	1.102428	-0.232147
6	0	-0.244819	1.255606	-1.417549
6	0	-0.196422	1.705297	0.834301
6	0	-1.439917	1.944216	-1.082286
1	0	0.030552	0.896398	-2.400170
6	0	-1.410981	2.220972	0.310964
1	0	0.102166	1.710179	1.874399
1	0	-2.243485	2.188921	-1.762865
1	0	-2.193973	2.703663	0.879238
6	0	1.840280	0.423935	-0.122133
6	0	2.159256	-0.670233	-0.937533
6	0	2.793980	0.873133	0.798331
6	0	3.397813	-1.296558	-0.834820
1	0	1.418459	-1.042011	-1.641472
6	0	4.030878	0.241409	0.908049
1	0	2.567361	1.735270	1.419104
6	0	4.338656	-0.844850	0.091456
1	0	3.627073	-2.145391	-1.472016
1	0	4.758708	0.605678	1.626666
1	0	5.303141	-1.335730	0.174898
1	0	-3.813784	-0.336955	1.376994

R) 1-([1,1'-Biphenyl]-4-yl)ferrocene

6	0	-2.870294	-2.066768	-0.800315
6	0	-2.150395	-2.018099	0.424105
6	0	-3.064997	-1.678807	1.456886
6	0	-4.349894	-1.515867	0.871101
6	0	-4.229839	-1.755519	-0.524239
1	0	-2.450088	-2.267576	-1.776603
1	0	-1.084249	-2.160980	0.541261
1	0	-2.818282	-1.531054	2.499130
1	0	-5.024528	-1.677489	-1.253108
26	0	-2.992990	-0.110016	0.021293
6	0	-1.433519	1.322912	-0.200084
6	0	-2.261355	1.325433	-1.362116
6	0	-2.258409	1.681390	0.906901
6	0	-3.578691	1.681397	-0.973081
1	0	-1.936766	1.085890	-2.365812
6	0	-3.577755	1.900000	0.430583
1	0	-1.941912	1.718258	1.940946
1	0	-4.437725	1.743827	-1.626464
1	0	-4.437970	2.150327	1.035806
6	0	-0.000016	0.977407	-0.150360
6	0	0.556797	0.069530	-1.061241
6	0	0.844176	1.554501	0.804234
6	0	1.909310	-0.246156	-1.020314
1	0	-0.087566	-0.416103	-1.789973
6	0	2.196532	1.231130	0.851141
1	0	0.441580	2.283996	1.501101
6	0	2.754420	0.326831	-0.060399
1	0	2.311150	-0.973881	-1.719931
1	0	2.837021	1.713404	1.584440
6	0	4.197466	-0.014260	-0.008512
6	0	4.942232	-0.171872	-1.184399
6	0	4.846837	-0.184280	1.221067
6	0	6.297153	-0.489352	-1.132041
1	0	4.460460	-0.018557	-2.146069
6	0	6.202032	-0.499084	1.274707
1	0	4.277427	-0.092233	2.141818
6	0	6.932907	-0.653560	0.097695
1	0	6.859340	-0.598712	-2.054479
1	0	6.685184	-0.633851	2.237611
1	0	7.989175	-0.900236	0.137976
1	0	-5.252690	-1.226079	1.390801

S) 1-(4-Methoxyphenyl)ferrocene

6	0	-2.343208	1.875627	-0.979869
6	0	-2.275999	2.114743	0.418368
6	0	-0.991016	1.712275	0.869982
6	0	-0.254023	1.221333	-0.247108
6	0	-1.100528	1.324646	-1.390103
1	0	-3.199627	2.053293	-1.615537
1	0	-3.075973	2.495455	1.038042
1	0	-0.645515	1.718703	1.895457
1	0	-0.836595	1.024773	-2.395521
26	0	-2.006146	0.035156	0.037064
6	0	-3.563695	-1.130591	0.905977
6	0	-3.461530	-1.433303	-0.478608
6	0	-2.324304	-1.457329	1.519402
6	0	-2.158501	-1.948001	-0.719659

1	0	-4.227933	-1.270040	-1.223554
6	0	-1.454873	-1.961248	0.514750
1	0	-2.072283	-1.309500	2.560398
1	0	-1.762482	-2.246865	-1.680672
6	0	1.120966	0.684582	-0.222268
6	0	1.507579	-0.366359	-1.069818
6	0	2.081576	1.216371	0.636739
6	0	2.800728	-0.861102	-1.056674
1	0	0.771960	-0.809648	-1.736603
6	0	3.389100	0.725251	0.668974
1	0	1.813869	2.045739	1.285384
6	0	3.751775	-0.317409	-0.183507
1	0	3.102434	-1.676014	-1.706425
1	0	4.105596	1.168619	1.350272
8	0	4.993335	-0.870868	-0.240468
6	0	5.991668	-0.330416	0.598536
1	0	5.726093	-0.444002	1.656709
1	0	6.899620	-0.895462	0.390082
1	0	6.163049	0.730204	0.377881
1	0	-0.422699	-2.254161	0.654868
1	0	-4.420691	-0.692635	1.398642

T) 4-(Ferrocen-1-yl)benzaldehyde

6	0	2.286416	1.862245	0.985792
6	0	2.229201	2.100159	-0.413845
6	0	0.942629	1.717683	-0.871968
6	0	0.195369	1.234008	0.242626
6	0	1.037790	1.326515	1.391347
1	0	3.141416	2.031824	1.625392
1	0	3.037398	2.469377	-1.029670
1	0	0.603936	1.730055	-1.899475
1	0	0.766146	1.034590	2.396804
26	0	1.925273	0.020484	-0.031877
6	0	3.450775	-1.162990	-0.926803
6	0	3.381787	-1.450066	0.463112
6	0	2.193869	-1.487509	-1.505120
1	0	4.297874	-0.736209	-1.445686
6	0	2.081575	-1.952501	0.743011
1	0	4.167486	-1.283248	1.186835
6	0	1.347192	-1.974424	-0.473376
1	0	1.916493	-1.350244	-2.541080
1	0	1.708335	-2.238281	1.716953
6	0	-1.180980	0.707353	0.211238
6	0	-1.590839	-0.287367	1.110040
6	0	-2.108931	1.204219	-0.718639
6	0	-2.893190	-0.770390	1.080022
1	0	-0.874142	-0.693635	1.818586
6	0	-3.407359	0.716734	-0.755696
1	0	-1.804886	1.991855	-1.401568
6	0	-3.806941	-0.274332	0.146298
1	0	-3.204961	-1.544425	1.778113
1	0	-4.132826	1.096407	-1.469001
6	0	-5.190047	-0.800783	0.121811
8	0	-6.048857	-0.430482	-0.647264
1	0	-5.408836	-1.584808	0.876608
1	0	0.310429	-2.263313	-0.584984

U) 1,1'-Diphenylferrocene (unfolded)

6	0	0.036225	2.084292	-1.269173
6	0	-0.332782	2.086954	0.103074
6	0	0.739928	1.525727	0.844490
6	0	1.778455	1.167252	-0.064730
6	0	1.333790	1.517372	-1.374186
1	0	-0.574779	2.424612	-2.094003
1	0	-1.284236	2.407564	0.506029
1	0	0.745495	1.338727	1.910203
1	0	1.890413	1.366224	-2.289263
26	0	0.006426	0.085386	-0.539519
6	0	-1.760726	-1.088955	-0.314851
6	0	-1.309449	-1.146880	-1.666646
6	0	-0.720557	-1.621902	0.502041
6	0	-0.006164	-1.710858	-1.678446
1	0	-1.868679	-0.812648	-2.530363
6	0	0.359356	-2.002171	-0.336717
1	0	-0.731659	-1.666413	1.583122
1	0	0.609743	-1.865713	-2.553872
6	0	3.057127	0.512530	0.278609
6	0	3.666196	-0.381099	-0.612723
6	0	3.688581	0.773069	1.500083
6	0	4.870634	-0.998393	-0.291272
1	0	3.174839	-0.607711	-1.555780
6	0	4.890899	0.148704	1.826714
1	0	3.240175	1.481345	2.191071
6	0	5.487430	-0.738468	0.933046
1	0	5.324358	-1.691643	-0.993086
1	0	5.366287	0.362377	2.779251
1	0	6.424382	-1.223914	1.187066
1	0	1.314424	-2.388393	-0.005831
6	0	-3.056724	-0.560877	0.155390
6	0	-3.691909	0.498168	-0.506890
6	0	-3.683522	-1.124384	1.272427
6	0	-4.921124	0.978270	-0.064224
1	0	-3.204685	0.957629	-1.363636
6	0	-4.909723	-0.638722	1.721598
1	0	-3.212258	-1.960928	1.780443
6	0	-5.534183	0.413355	1.054599
1	0	-5.398638	1.800797	-0.588093
1	0	-5.381910	-1.089975	2.588874
1	0	-6.490895	0.790108	1.402074

V) 1,1'-Bis([1,1'-diphenyl]-4-yl)ferrocene (unfolded)

6	0	-0.276260	-2.679377	-1.054009
6	0	-0.689434	-1.438814	-1.609690
6	0	0.434569	-0.572865	-1.630219
6	0	1.553263	-1.272219	-1.086110
6	0	1.103688	-2.578721	-0.733414
1	0	-0.909660	-3.535846	-0.867541
1	0	-1.693523	-1.180855	-1.919134
1	0	0.443026	0.449041	-1.984768
1	0	1.699805	-3.339276	-0.246703
26	0	0.008622	-1.126667	0.373969
6	0	-1.531597	-0.284540	1.583100
6	0	-1.082271	-1.510991	2.156759
6	0	-0.412391	0.599277	1.545309
6	0	0.296653	-1.380794	2.467706

1	0	-1.692013	-2.390104	2.317487
6	0	0.711946	-0.076782	2.087576
1	0	-0.412489	1.594298	1.119343
1	0	0.928900	-2.150392	2.888161
6	0	2.910710	-0.728308	-0.887392
6	0	4.034456	-1.558898	-0.954529
6	0	3.110974	0.634538	-0.630984
6	0	5.314098	-1.047642	-0.759490
1	0	3.904199	-2.616124	-1.167564
6	0	4.388900	1.146132	-0.443161
1	0	2.250998	1.296758	-0.566226
6	0	5.514233	0.312636	-0.498563
1	0	6.169597	-1.716714	-0.791282
1	0	4.521012	2.209807	-0.264865
1	0	1.719678	0.311872	2.149549
6	0	-2.893125	0.003550	1.092622
6	0	-3.699323	-1.010719	0.559569
6	0	-3.418715	1.298506	1.158669
6	0	-4.987190	-0.739683	0.114577
1	0	-3.297043	-2.016668	0.467234
6	0	-4.705213	1.571480	0.704729
1	0	-2.822313	2.093860	1.596778
6	0	-5.513772	0.557685	0.178461
1	0	-5.584321	-1.537134	-0.319281
1	0	-5.102984	2.578590	0.794268
6	0	6.877160	0.857456	-0.280658
6	0	7.955092	0.433585	-1.068334
6	0	7.113597	1.806935	0.722009
6	0	9.233554	0.944500	-0.859195
1	0	7.783165	-0.284343	-1.865474
6	0	8.391393	2.318818	0.931549
1	0	6.291966	2.126487	1.357131
6	0	9.456623	1.889280	0.141570
1	0	10.055697	0.611237	-1.485167
1	0	8.556486	3.048459	1.718349
1	0	10.452858	2.288568	0.303603
6	0	-6.891693	0.846500	-0.290332
6	0	-7.938957	-0.043790	-0.020099
6	0	-7.176188	2.016369	-1.006305
6	0	-9.234082	0.227432	-0.453287
1	0	-7.738472	-0.942491	0.556612
6	0	-8.471333	2.289360	-1.438629
1	0	-6.370026	2.704871	-1.244272
6	0	-9.505468	1.395684	-1.163711
1	0	-10.034698	-0.470286	-0.227427
1	0	-8.672194	3.197881	-1.998135
1	0	-10.515217	1.608367	-1.500441

W) 1,1'-Bis(4-methoxyphenyl)ferrocene (unfolded)

6	0	-0.226660	-0.767438	2.351736
6	0	-0.540230	-1.543515	1.203869
6	0	0.612585	-1.582587	0.375351
6	0	1.646574	-0.828593	1.004077
6	0	1.117635	-0.325271	2.229321
1	0	-0.901266	-0.527465	3.162433
1	0	-1.503760	-1.978708	0.973563
1	0	0.681426	-2.050008	-0.598246
1	0	1.653220	0.293749	2.936729
26	0	-0.029438	0.433720	0.610157

6	0	-1.685630	1.357830	-0.365938
6	0	-1.253699	2.166705	0.726411
6	0	-0.589987	1.251838	-1.272119
6	0	0.093316	2.553435	0.491962
1	0	-1.852910	2.431372	1.587317
6	0	0.504845	1.985457	-0.743394
1	0	-0.579362	0.658024	-2.176659
1	0	0.705444	3.152004	1.152759
6	0	3.007291	-0.600253	0.479952
6	0	3.676446	0.616037	0.693598
6	0	3.675856	-1.597078	-0.229063
6	0	4.960854	0.821642	0.218897
1	0	3.167265	1.416331	1.225350
6	0	4.968838	-1.404885	-0.721659
1	0	3.188064	-2.554716	-0.388168
6	0	5.616314	-0.190336	-0.494416
1	0	5.479262	1.761470	0.377615
1	0	5.454751	-2.207918	-1.262988
8	0	6.873177	0.105068	-0.923399
6	0	7.563814	-0.881616	-1.659798
1	0	7.027326	-1.136454	-2.581845
1	0	8.531801	-0.448802	-1.910745
1	0	7.714461	-1.789851	-1.063392
1	0	1.493597	2.054106	-1.177389
6	0	-3.009631	0.722883	-0.519080
6	0	-3.730344	0.267710	0.585921
6	0	-3.586448	0.566134	-1.788256
6	0	-4.987269	-0.322996	0.449125
1	0	-3.293162	0.356847	1.577675
6	0	-4.830331	-0.026003	-1.944094
1	0	-3.054410	0.928789	-2.663343
6	0	-5.540434	-0.473016	-0.824723
1	0	-5.511931	-0.664862	1.333412
1	0	-5.280694	-0.146709	-2.923830
8	0	-6.753038	-1.037027	-1.075624
6	0	-7.497336	-1.509019	0.026805
1	0	-8.419315	-1.919387	-0.383835
1	0	-6.955000	-2.296610	0.563951
1	0	-7.738734	-0.694647	0.720827

X) 4,4'-(Ferrocen-1,1'-diyl)dibenzaldehyde (unfolded)

6	0	0.098237	-1.049461	2.470791
6	0	0.545740	0.237391	2.067775
6	0	-0.520357	0.877685	1.384799
6	0	-1.634213	-0.013713	1.354139
6	0	-1.240954	-1.207411	2.030551
1	0	0.685394	-1.791702	2.993406
1	0	1.540408	0.638939	2.208838
1	0	-0.479641	1.851653	0.914503
1	0	-1.861051	-2.081691	2.177062
26	0	0.020308	-0.901396	0.348510
6	0	1.674466	-1.019684	-0.986964
6	0	1.309265	-2.331695	-0.564394
6	0	0.546351	-0.459872	-1.659363
6	0	-0.028364	-2.574982	-0.971081
1	0	1.928290	-2.999497	0.019998
6	0	-0.498363	-1.418569	-1.650481
1	0	0.496803	0.529604	-2.093720
1	0	-0.600817	-3.468390	-0.762896

6	0	-2.940980	0.240292	0.721050
6	0	-3.693841	-0.811364	0.180439
6	0	-3.457922	1.544339	0.663275
6	0	-4.931411	-0.564365	-0.400783
1	0	-3.291833	-1.820877	0.201424
6	0	-4.689373	1.793957	0.074702
1	0	-2.891603	2.359829	1.103162
6	0	-5.434114	0.737846	-0.459437
1	0	-5.510468	-1.383883	-0.821108
1	0	-5.099188	2.798472	0.026264
6	0	-6.751387	0.989190	-1.086963
8	0	-7.261394	2.082473	-1.189018
1	0	-7.268503	0.087065	-1.475361
1	0	-1.490839	-1.275716	-2.056578
6	0	2.967808	-0.353392	-0.748036
6	0	4.147742	-1.104194	-0.685859
6	0	3.041449	1.041905	-0.589597
6	0	5.370119	-0.478038	-0.463433
1	0	4.105182	-2.179181	-0.831801
6	0	4.259026	1.667844	-0.375542
1	0	2.126432	1.627888	-0.616166
6	0	5.432867	0.907187	-0.308836
1	0	6.283882	-1.066635	-0.419644
1	0	4.327604	2.744246	-0.248598
6	0	6.739085	1.563360	-0.074311
8	0	6.885684	2.755236	0.080351
1	0	7.612347	0.878967	-0.045355