A chelating bis(aminophenol) ligand bridged by a 1,1'-ferrocenebis(*para*-phenylene) linker

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I. Hammett plots of substituent effects on redox potentials of substituted ferrocenes and arylferrocenes





II. Cyclic voltammograms of Fe(C₅H₄C₆H₄NH₂)₂ and *p*FlipH₄

Conditions: CH_2Cl_2 , 1 mM analyte, 100 mM [Bu₄N]PF₆ supporting electrolyte, scan rate 120 mV s⁻¹.

II. NMR spectra of (*p*Flip)Pd (CD₂Cl₂)

(a) 1 H NMR



III. Energy and Cartesian coordinates of (*p*Flip*)Pd

Energy of optimized structure = -2961.57397513 a.u.

Center	Atomic	Coor	dinates (Ang	gstroms)
Number	Number	Х	Y	Z
	46		0 000026	0 000029
2	8	-4.588801	-1.410071	0.029191
3	7	-1.995550	-1.651078	-0.067946
4	6	-4.136049	-2.631570	0.024442
5	6	-4.996560	-3.754319	0.054963
6	1	-6.066997	-3.581224	0.099974
7	6	-4.456662	-5.024484	0.020119
8	1	-5.111759	-5.890927	0.042055
9	6	-3.052823	-5.213522	-0.057410
10	1	-2.652482	-6.222287	-0.103809
11	6	-2.187088	-4.138729	-0.084104
12	1	-1.117466	-4.295621	-0.157287
13	6	-2.707367	-2.815960	-0.026459
14	8	-4.588768	1.410149	-0.029268
15	7	-1.995520	1.651091	0.068062
16	6	-4.135981	2.631640	-0.024510
17	6	-4.996452	3.754415	-0.055127
18	1	-6.066892	3.581356	-0.100227
19	6	-4.456515	5.024563	-0.020248
20	1	-5.111583	5.891026	-0.042250
21	6	-3.052678	5.213562	0.057413
22	1	-2.652315	6.222317	0.103849
23	6	-2.186975	4.138745	0.084194
24	1	-1.117355	4.295600	0.157485
25	6	-2.707293	2.815997	0.026500
26	26	4.929699	-0.000007	0.000000
27	6	3.721898	-1.686226	-0.187937
28	6	4.585787	-1.787327	0.956088
29	1	4.266094	-1.891664	1.984372
30	6	5.939464	-1.713077	0.516194
31	1	6.816054	-1.755152	1.149321
32	6	5.932001	-1.548456	-0.900962
33	I C	6.801920	-1.451908	-1.53/320
34	0	4.5/4231	-1.521098	-1.333/4/
35		4.244545	-1.419/59	-2.339000
30	6	2.250009	-1./434/5	-0.182815
20	0	1.49/124	-1.249130	-1.202003
20	1	2.004/00	-0.043412	-2.132133
39	0	0.108000	-1.22/524	-1.22004/
40	1	0 580/72	1 713004	-2.030934
42	6	0.156848	-2.249514	0.960419
42	1	-0.369207	-2.638710	1.827357
44	- 6	3,721921	1.686194	0.187932
45	6	4.585747	1.787265	-0.956133
46	1	4.266012	1.891527	-1.984412
47	- 6	5,939442	1.713052	-0.516290
48	1	6.816010	1.755117	-1.149448
-				

Cartesian coordinates of optimized structure:

49	6	5.932050	1.548469	0.900868
50	1	6.801996	1.451972	1.537197
51	6	4.574293	1.521117	1.333712
52	1	4.244638	1.419813	2.359043
53	6	2.250694	1.743414	0.182832
54	6	1.497186	1.248913	1.262624
55	1	2.004865	0.843056	2.132013
56	6	0.108672	1.227275	1.226645
57	1	-0.459681	0.823780	2.058909
58	6	-0.580431	1.712928	0.106773
59	6	0.156847	2.249563	-0.960280
60	1	-0.369244	2.638884	-1.827142
61	6	1.547650	2.262574	-0.918491
62	1	2.095935	2.679994	-1.757894
63	6	1.547654	-2.262516	0.918581
64	1	2.095969	-2.679821	1.758022