# Supplementary Material (ESI) for Chemical Communications

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### **EXPERIMENTAL**

**General**: Pyridine, *d*-chloroform and acetonitrile was dried over 3Å molecular sieves. Tetra-*n*-butylammonium salts were dried under a vacuum at 50°C and stored in a desicator. All other materials were obtained from TCI-America, Sigma-Aldrich, Acros and Strem. Nuclear Magnetic Resonance <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR spectra were recorded on a Varian INOVA 300 (299.935), 125 (125.751) and 282 (282.224) MHz spectrometer respectively. Chemical shifts ( $\delta$ ) expressed as ppm downfield from tetramethylsilane using either the residual solvent peak as an internal standard (CDCl<sub>3</sub> <sup>1</sup>H: 7.27 ppm) or using CDCl<sub>3</sub> spiked with 1% trimethylsilane for the <sup>1</sup>H NMR spectra. For the <sup>13</sup>C NMR spectra the middle CDCl<sub>3</sub> peak ( $\delta$  77.00 ppm) was used as the internal standard Signal patterns are indicated as b, broad; s, singlet; d, doublet; t, triplet; m, multiplet. Coupling constants (*J*) are given in hertz.

Single-crystal X-ray diffraction data for compounds 1 and  $1 \cdot nBu_4^+ \cdot Cl^-$  were collected on a Bruker-AXS SMART APEX/CCD diffractometer using Mo<sub>ka</sub> radiation ( $\lambda = 0.7107$  Å) at 152 K. Diffracted data have been corrected for Lorentz and polarization effects, and for absorption using the SADABS v2.02 area-detector absorption correction program (Siemens Industrial Automation, Inc., © 1996). The structures were solved by direct methods and the structure solution and refinement was based on  $|F|^2$ . All non-hydrogen atoms were refined with anisotropic displacement parameters whereas hydrogen atoms were placed in calculated positions when possible and given isotropic U values 1.2 times that of the atom to which they are bonded. Hydrogen atoms of the amino groups in 1 and  $1 \cdot nBu_4^+ \cdot Cl^-$  were located via difference Fourier map inspection and refined with riding coordinates and isotropic thermal parameters based upon the corresponding N atoms [U(H) = 1.2Ueq (O)]. All crystallographic calculations were conducted with the SHELXTL v.6.1 program package (Bruker AXS Inc., © 2001).

2-p-toluenesulfonamide-2', 3', 4', 5', 6'-pentafluorobiphenyl (1). An oven dried 100 mL round bottom Schlenk flask was charged with N-(2-iodophenyl)-4-methylbenzenesulfonamide (3.68 g, 14.9 mmol), copper powder (4.77 g, 75.1 mmol) and tetrakistriphenylphosphine palladium (0) (0.860 g, 0.741 mmol). Dry dimethylsulfoxide (46 mL) was added via a syringe to the reaction mixture. The mixture was degassed purging with  $N_2$  (3×) and then bromopentafluorobenzene (3.70 mL, 29.7 mmol) was added. The solution was again degassed and then was heated at 115- $120^{\circ}$ C for 5.5 h. under a N<sub>2</sub> atmosphere. The reaction was cooled to room temperature and was diluted with DCM (50 mL) and water (50 mL). The resulting foamy mixture was then filtered through a glass frit containing celite and silica gel. The remaining celite/silica gel pad was washed with DCM ( $3 \times 50$  mL). The resulting pale green solution was transferred to a 150 mL separatory funnel and washed with water (3  $\times$  100 mL) followed by brine (1  $\times$  100 mL). The separated organic layer was dried over MgSO<sub>4</sub>. Removal of the DCM in vacuo left a crude pale green solid that was later purified by flash column chromatography (silica gel, 3:1 hexanes: ethyl acetate) to yield a colorless product (1.64 g, 26.7% yield) that crystallized overnight upon standing in the column eluent. Structure was determined by single crystal X-ray diffraction. Single crystals suitable for data collection were grown by diffusing pentane into a chloroform solution of 1 at  $-30^{\circ}$ C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>; 25°C):  $\delta$  7.56 (d, J = 8.1 Hz, 1H, CH), 7.48 (t, J = 4.5 Hz, 1H, ArCH), 7.41 (d, J = 4.6 Hz, 2H, ArCH), 7.35 (t, J = 4.2 Hz, 1H, ArCH), 7.17 (m, 3H, ArC*H*), 6.35 (b, 1H, N*H*), 2.41 (s, 3H, C*H*<sub>3</sub>); <sup>19</sup>F NMR (282 MHz, CDCl<sub>3</sub>; 25°C):  $\delta$  – 191.51 (q, *J* = 16.2 Hz, 2F C*F*), -205.54 (t, *J* = 22.2 Hz, 1F, C*F*), -213.14 (m, 2F, C*F*). <sup>13</sup>C NMR

(125 MHz, CDCl<sub>3</sub>; 25°C):  $\delta$  144.37, 144.45, 136.36, 134.57, 131.90, 131.04, 129.73, 127.39, 127.25, 127.04, 122.46, 21.62, 0.202.

*N*-biphenyl-2-yl-4-methyl-benzenesulfonamide (2). Similar to literature procedure,<sup>1</sup> an oven dried 50 mL round bottom flask was charged with 2-aminobiphenyl (0.330 g, 2.00 mmol) and pyridine (7.5 mL). To this stirred solution *p*-toluenesulfonylchloride (0.570 g, 3.00 mmol) was added and stirred for 4 h. The resulting pale pink solution with white precipitate was concentrated down in vacuo and diluted with dichloromethane (50 mL) and water (50 mL). The organic layer was separated and washed with 3M HCl ( $3 \times 50$  mL) and 1M NaHCO<sub>3</sub> ( $3 \times 50$  mL). Removal of the organic layer in vacuo resulted in a pale pink solid that was later crystallized from an 8:1 mixture of hexanes and dichloromethane. Crystallization yielded colorless crystals (0.56 g, 87%). The structure was determined by single crystal X-ray diffraction. Single crystals suitable for data collection were grown by diffusing pentane into a chloroform solution of **2** at  $-30^{\circ}$ C. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>; 25°C):  $\delta$  7.80 (d, *J* = 8.1 Hz, 2H, ArC*H*), 7.72 (d, *J* = 8.1 Hz, 1H, ArC*H*), 7.48 (d, *J* = 8.7 Hz, 1H, ArC*H*), 7.35 (m, 4H, ArC*H*), 7.20 (d, *J* = 8.4 Hz, 2H, ArC*H*), 7.12 (m, 1H, ArC*H*), 6.86 (m, 2H, ArC*H*), 6.58 (b, 1H, N*H*), 2.41 (s, 3H, C*H*<sub>3</sub>).

### NMR Studies:

<sup>1</sup>H NMR spectra were recorded on a Varian 300 or 500 MHz spectrometer. Each titration was performed with 8 to 14 measurements in CDCl<sub>3</sub> at room temperature. CDCl<sub>3</sub> was passed through activated alumina and dried over 3Å molecular sieves. Aliquots from a stock solution of tetra-*n*-butylammonium salts (60 – 200 mM) were added to the initial solution of receptor (9 – 25 mM). All additions were done through septa with a syringe to minimize evaporation. All proton signals were referenced to an internal TMS standard. The association constants Ka were calculated by the non-linear regression curve fitting program WinEQNMR

		fromGuest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.2480	0	0.6	9.677E-03	0.000E+00
1	6.3005	0.01	0.61	9.518E-03	1.039E-03
2	6.3483	0.02	0.62	9.365E-03	2.044E-03
3	6.3937	0.03	0.63	9.216E-03	3.017E-03
4	6.4360	0.04	0.64	9.072E-03	3.960E-03
5	6.5128	0.06	0.66	8.797E-03	5.760E-03
6	6.5816	0.08	0.68	8.538E-03	7.455E-03
7	6.6474	0.1	0.7	8.294E-03	9.052E-03
8	6.7038	0.12	0.72	8.064E-03	1.056E-02
9	6.7789	0.15	0.75	7.741E-03	1.267E-02
10	6.8479	0.18	0.78	7.444E-03	1.462E-02
11	6.9067	0.21	0.81	7.168E-03	1.643E-02
12	6.9735	0.25	0.85	6.831E-03	1.864E-02
13	7.0401	0.3	0.9	6.451E-03	2.112E-02
14	7.1055	0.35	0.95	6.112E-03	2.334E-02

<sup>1</sup>H NMR Titration data for receptor 1 and TBACl trial 1:

mol Receptor

initial vol. (G) Receptor Stock (M) Guest Stock (M) Mol Guest 0.6 0.009676678 0.063363558 0.000126727

9.67668E-06 **TBACI MW** Receptor 2 MW 413.365 277.92 4.0 10\*\*3 Res -4.0 8.0 7.6  $K_1 = 24.1 + - 0.8$ [shift]/10\*\* 0 7.2 6.8 6.4 6.0 0.0 15.6 26.0 10.4 20.8 5.2 10\*\*3[Concentration]/mol dm-3 Measured Chemical shifts for a 1:1 complex [0075]

### <sup>1</sup>H NMR Titration data for receptor 1 and TBACl trial 2:

		from Guest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.2414	0	0.6	9.822E-03	0.000E+00
1	6.2950	0.01	0.61	9.661E-03	9.874E-04
2	6.3465	0.02	0.62	9.505E-03	1.943E-03
3	6.3969	0.03	0.63	9.354E-03	2.868E-03
4	6.4392	0.04	0.64	9.208E-03	3.765E-03
5	6.5203	0.06	0.66	8.929E-03	5.476E-03
6	6.5929	0.08	0.68	8.666E-03	7.086E-03
7	6.6544	0.1	0.7	8.419E-03	8.605E-03
8	6.7396	0.13	0.73	8.073E-03	1.073E-02
9	6.8080	0.16	0.76	7.754E-03	1.268E-02
10	6.8934	0.2	0.8	7.366E-03	1.506E-02
11	6.9692	0.25	0.85	6.933E-03	1.772E-02
12	7.0955	0.35	0.95	6.203E-03	2.219E-02

initial vol. (R)	Receptor Stock (M)	Guest Stock (M)	mol Guest (G)
0.6	0.009821828	0.060233161	0.000120466
	mol Receptor		
	9.82183E-06		
	TBACI MW	Receptor 2 MW	
	277.92	413.365	



H NMF	R Titration da	ata for receptor 1 + T	BABr trial 1:		
		from Guest Stock			
Addition	δ ррт	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.2463	0	0.6	1.040E-02	0.000E+00
1	6.3003	0.01	0.61	1.023E-02	1.051E-03
2	6.3488	0.02	0.62	1.007E-02	2.069E-03
3	6.3962	0.03	0.63	9.907E-03	3.054E-03
4	6.4799	0.05	0.65	9.602E-03	4.934E-03
5	6.5543	0.07	0.67	9.316E-03	6.701E-03
6	6.6207	0.09	0.69	9.046E-03	8.366E-03
7	6.6811	0.11	0.71	8.791E-03	9.937E-03
8	6.7608	0.14	0.74	8.434E-03	1.213E-02
9	6.8279	0.17	0.77	8.106E-03	1.416E-02
10	6 9045	0.21	0.81	7 706E-03	1 663E-02

0.86

0.96

7.258E-03

6.502E-03

0.26

0.36

1.939E-02

2.405E-02

1

11

12

6.9863

7.1104

initial vol. (R)	Receptor Stock (M)	Guest Stock (M)	mol Guest (G)
0.6	0.010402429	0.064137162	0.000128274
	mol Receptor		
	1.04024E-05		
	TBACI MW	Receptor 2 MW	
	277.92	413.365	



<sup>1</sup> H NMR Titration data for receptor 1 + TBABr tr	ial 1:
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		from Guest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.358	0	0.6	2.035E-02	0.000E+00
1	6.359	0.01	0.61	2.001E-02	3.260E-03
2	6.453	0.03	0.63	1.938E-02	9.470E-03
3	6.53	0.05	0.65	1.878E-02	1.530E-02
4	6.593	0.07	0.67	1.822E-02	2.078E-02
5	6.67	0.1	0.7	1.744E-02	2.841E-02
6	6.736	0.13	0.73	1.672E-02	3.541E-02
7	6.785	0.16	0.76	1.606E-02	4.187E-02
8	6.847	0.2	0.8	1.526E-02	4.972E-02
9	6.91	0.25	0.85	1.436E-02	5.849E-02
10	7.019	0.35	0.95	1.285E-02	7.327E-02
11	7.086	0.45	1.05	1.163E-02	8.523E-02



<sup>1</sup>H NMR Titration data for receptor 1 + TBABr trial 2:

		from Guest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.284	0	0.6	0.01982719	0
1	6.315	0.01	0.61	0.019502154	0.001980689
2	6.327	0.02	0.62	0.019187603	0.003897485
3	6.346	0.04	0.64	0.018587991	0.007551377
4	6.365	0.06	0.66	0.018024718	0.01098382
5	6.389	0.09	0.69	0.017241035	0.015759394
6	6.409	0.12	0.72	0.016522658	0.020137004
7	6.431	0.16	0.76	0.015653045	0.025436216
8	6.45	0.21	0.81	0.014686807	0.031324228
9	6.477	0.31	0.91	0.013072872	0.041159151

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initial vol. (R)	Receptor Stock (M)	Guest Stock (M)	mol Guest
0.6	1.98E-02	0.120822024	0.000241644
	mol Receptor		
	1.98E-05		
	TBABr MW	Receptor MW	
	322.375	413.365	



		1			
		from Guest Stock			
Addition	δ ppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.297	0	0.6	2.032E-02	0
1	6.299	0.01	0.61	1.999E-02	0.001977638
2	6.366	0.02	0.62	1.967E-02	0.003891481
3	6.398	0.03	0.63	1.935E-02	0.005744567
4	6.452	0.05	0.65	1.876E-02	0.009279685
5	6.497	0.07	0.67	1.820E-02	0.012603751
6	6.557	0.1	0.7	1.742E-02	0.017233701
7	6.606	0.13	0.73	1.670E-02	0.021483106
8	6.659	0.17	0.77	1.583E-02	0.026633901
9	6.710	0.22	0.82	1.487E-02	0.032365731
10	6.793	0.32	0.92	1.325E-02	0.041960315

<sup>1</sup>H NMR Titration data for receptor 1 + TBABr trial 3:

initial vol. (R)	Receptor Stock (M)	Guest Stock (M)	mol Guest
0.6	2.03E-02	0.120635905	0.000241272
	mol Receptor		
	2.03E-05		
	TBABr MW	Receptor MW	
	322.375	413.365	



<sup>1</sup> H NMR	titration	data	for rece	ptor 1 -	+ TBAI	trial	1:
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		1			
		from Guest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.295	0	0.6	0.019111439	0.0000E+00
1	6.309	0.01	0.61	0.018798137	1.9872E-03
2	6.329	0.03	0.63	0.018201371	5.7724E-03
3	6.356	0.06	0.66	0.017374035	1.1020E-02
4	6.377	0.09	0.69	0.016618643	1.5811E-02
5	6.392	0.12	0.72	0.015926199	2.0203E-02
6	6.405	0.15	0.75	0.015289151	2.4244E-02
7	6.42	. 0.19	0.79	0.014515017	2.9154E-02
8	6.435	0.24	0.84	0.013651028	3.4634E-02
9	6.445	0.28	0.88	0.013030527	3.8570E-02
10	6.457	0.35	0.93	0.012329961	4.5620E-02

-			
initial vol. (G)	Receptor Stock (M)	Guest Stock (M)	mol Guest
0.6	0.019111439	0.121219915	0.00024244
	mol Receptor		
	1.91114E-05		
	TBAI MW	Receptor MW	
	369.37	413.365	



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		from Guest Stock				
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]		[G]
0	6.303	0	0.6	2.032E-02		0.000E+00
1	6.318	0.01	0.61	1.999E-02		1.934E-03
2	6.336	0.03	0.63	1.935E-02		5.616E-03
3	6.361	0.06	0.66	1.847E-02		1.072E-02
4	6.378	0.09	0.69	1.767E-02		1.538E-02
5	6.393	0.12	0.72	1.693E-02		1.966E-02
6	6.404	0.15	0.75	1.626E-02		2.359E-02
7	6.417	0.19	0.79	1.543E-02		2.837E-02
8	6.431	0.24	0.84	1.452E-02		3.370E-02
9	6.442	0.28	0.88	1.386E-02		3.753E-02

Η	NMR	titration	data	for	receptor	1 +	TBAI	trial 2	2
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		from Guest Stock			
Addition	δppm	Vol. Guest added (ml)	Total Vol. (ml)	[R]	[G]
0	6.293	0	0.6	0.019498506	0.0000E+00
1	6.306	0.01	0.61	0.019178859	1.9675E-03
2	6.326	0.03	0.63	0.018570006	5.7150E-03
3	6.344	0.05	0.65	0.017998621	9.2319E-03
4	6.364	0.08	0.68	0.017204564	1.4119E-02
5	6.379	0.11	0.71	0.016477611	1.8594E-02
6	6.395	0.14	0.74	0.0158096	2.2706E-02
7	6.41	0.18	0.78	0.014998851	2.7696E-02
8	6.421	0.23	0.83	0.014095306	3.3257E-02
9	6.442	0.28	0.88	0.013294436	3.8187E-02

initial vol			
(G)	Receptor Stock (M)	Guest Stock (M)	mol Guest
0.6	0.019498506	0.120015161	0.00024003
	mol Receptor		
	1.94985E-05		
	TBAI MW	Receptor MW	
	369.37	413.365	



### Dimerization Determination:

# <sup>1</sup>*H* NMR Dimerization data for receptor **1** trial 1:

		from Receptor Stock			
Addition	δppm	Vol. Receptor added (ml)	Total Vol. (ml)	[R]	[R] (M)
0	6.1908	0.01	0.61	2.652E-03	0.002651965
1	6.2100	0.02	0.62	5.218E-03	0.005218383
2	6.2435	0.04	0.64	1.011E-02	0.010110617
3	6.2751	0.06	0.66	1.471E-02	0.014706351
4	6.3008	0.08	0.68	1.903E-02	0.019031749
5	6.3251	0.1	0.7	2.311E-02	0.023109981
6	6.3469	0.12	0.72	2.696E-02	0.026961644
7	6.3655	0.14	0.74	3.061E-02	0.030605109
8	6.3881	0.17	0.77	3.572E-02	0.035715425
9	6.4129	0.2	0.8	4.044E-02	0.040442466
10	6.4394	0.24	0.84	4.622E-02	0.046219961
11	6.4686	0.29	0.89	5.271E-02	0.052711529
12	6.5101	0.39	0.99	6.373E-02	0.063727522
13	6.5453	0.49	1.09	7.272E-02	0.072722233
14	6.5718	0.59	1.19	8.021E-02	0.080205227

initial vol. (R)	Receptor Stock (M)		
0.61	0.161769864		
	mol Receptor		
	0.00016177		
		Receptor 1 MW	
		413.365	



		from Receptor Stock			
Addition	δppm	Vol. Receptor added (ml)	Total Vol. (ml)	[R]	[R] (M)
0	6.194	0.01	0.61	2.709E-03	0.00271
1	6.214	0.02	0.62	5.330E-03	0.00533
2	6.250	0.04	0.64	1.033E-02	0.01033
3	6.282	0.06	0.66	1.502E-02	0.01502
4	6.311	0.08	0.68	1.944E-02	0.01944
5	6.336	0.1	0.7	2.360E-02	0.02360
6	6.359	0.12	0.72	2.754E-02	0.02754
7	6.379	0.14	0.74	3.126E-02	0.03126
8	6.403	0.17	0.77	3.648E-02	0.03648
9	6.428	0.2	0.8	4.131E-02	0.04131
10	6.455	0.24	0.84	4.721E-02	0.04721
11	6.480	0.29	0.89	5.384E-02	0.05384
12	6.523	0.39	0.99	6.509E-02	0.06509
13	6.556	0.49	1.09	7.428E-02	0.07428
14	6.580	0.59	1.19	8.192E-02	0.08192

<sup>1</sup>*H* NMR Dimerization data for receptor **1** trial 2:

initial vol. (R)	Receptor Stock (M)		
0.61	0.165229277		
	mol Receptor		
	0.000165229		
		Receptor 1 MW	
		413.365	



### pKa determination:

The pKa measurements were made with an Orion model 230Aplus pH meter equipped with a Triode 9107BN pH electrode. The pH meter was calibrated with 1:1 stock solutions of acetonitrile/water buffered at 7.00 and 10.00 pH. The electrode was allowed to soak in acetonitrile for 2 hours prior to any measurements. Initial receptor concentrations were made to 10<sup>-3</sup> M in acetonitrile and 0.06 g tetra-*n*-butylammonium iodide was added as a supporting electrolyte. A stock solution of tetramethylammonium hydroxide in ethanol 0.05 M (to avoid precipitation) was prepared under nitrogen. Aliquots of the stock tetramethylammonium hydroxide were added to the receptor solution under nitrogen and the resulting potential was measured. Titration curves were prepared by plotting the potential vs the total amount of stock tetramethylammonium hydroxide added. The relative pKa was taken as the pH at the half-neutralization potential.

pKa determination for receptor 1:

11111 1			
Addition	Total Added	рН	RelmV
0	0	7.97	-99.6
1	50	8.51	-135.5
2	100	8.76	-150.7
3	150	8.89	-158.7
4	200	9	-165.8
5	250	9.09	-171.3
6	300	9.17	-176
7	350	9.24	-180.3
8	400	9.3	-183.9
9	450	9.36	-187.6
10	500	9.41	-190.8
11	750	9.66	-206.2
12	800	9.74	-210.7
13	850	9.84	-216.9
14	900	9.92	-221.6
15	950	10	-226.9
16	1000	10.09	-232.5
17	1050	10.18	-237.7
18	1100	10.45	-255.4
19	1150	10.8	-278.3
20	1200	13.45	-442.5
21	1250	13.85	-468.9
22	1300	14.26	-493.5
23	1400	14.47	-507.7
24	1600	14.98	-540.3
25	1900	15.36	-564.1

#### trial 1

 $HNP = -380 \text{ mV} = pH \ 13.3$ 





1	1
trial	
<i>ii iui</i>	4

Addition	Total Added	pН	RelmV
0	0	8.15	-101
1	30	9.39	-177.2
2	60	9.8	-202.6
3	90	10.19	-227.4
4	105	10.5	-246.5
5	115	10.88	-270.8
6	120	11.48	-308.6
7	125	13.52	-436.5
8	130	15.02	-532.3
9	140	17.46	-678
10	150	17.84	-711.3
11	165	18.18	-733.3
12	195	18.49	-753.7
13	245	18.67	-766.3
14	295	18.73	-769.8
15	345	18.72	-770.6

HNP = -505 mV = pH 14.2





PKa determination for Receptor 2:

Trial 1			
Addition	Total Added	pН	RelmV
0	0	8.56	-127.4
1	30	10.83	-268.2
2	40	10.97	-278
3	50	11.09	-286.2
4	55	11.15	-290.4
5	65	11.25	-297.6
6	75	11.35	-304.4
7	85	11.45	-311.4
8	100	11.62	-322.2
9	110	11.76	-331.9
10	120	11.95	-344.3
11	125	12.07	-352
12	130	12.27	-364.8
13	135	12.61	-386.8
14	140	13.17	-422.5
15	145	13.95	-472.8
16	150	14.5	-508.2
17	155	15.25	-556.6
18	160	16.36	-580.7
19	170	17.07	-666.8
20	180	17.6	-700
21	190	17.83	-720
22	200	17.93	-726

HNP = -540 mV = pH 15.1

# Supplem	entary Mate	rial (ESI) for	Chemical C	Communicati	ions
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23	220	18.04	-736.8
24	250	18.22	-747.5
25	300	18.35	-755.8
26	350	18.39	-757.7
27	400	18.39	-757.7



	7 · 1	<b>`</b>
1	rial	
1	iui	4

0	0	9.7	-201.8
1	20	10.76	-266.9
2	40	11.06	-285.7
3	60	11.28	-299.7
4	80	11.47	-312.2
5	100	11.68	-325.9
6	120	11.95	-343.6
7	130	12.16	-359.4
8	140	12.57	-385.3
9	150	13.65	-452.4
10	155	14.57	-510.2
11	160	16.3	-624
12	165	16.81	-652
13	170	17.12	-670.2
14	175	17.4	687.5
15	185	17.75	710.1

$$HNP = -550 \text{ mV} = pH \ 14.7$$

16	195	17.96	-724.3
17	215	18.15	-736.2
18	245	18.29	-745.5
19	295	18.38	-751.5
20	345	18.42	-753.8



1 Sakamoto, T.; Kondo, Y.; Iwashita, S.; Nagano, T.; Yamanaka, H. Chem. Pharm. Bull. 1988, 36, 1305-1308.