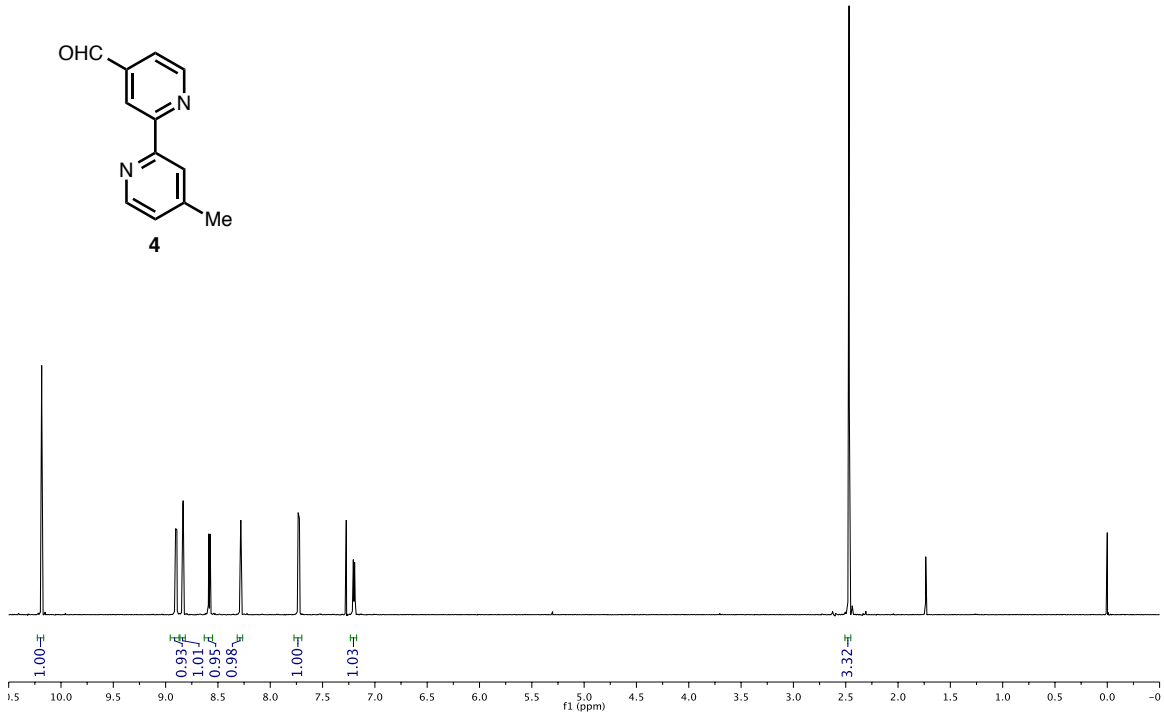
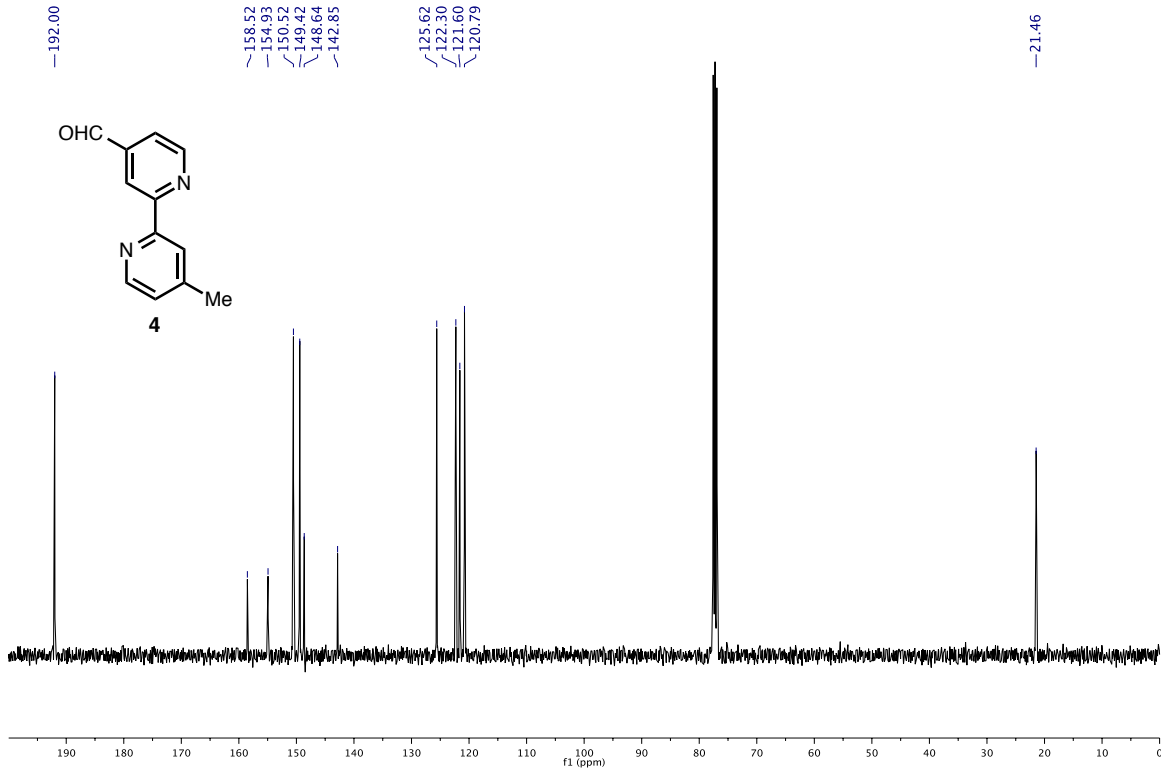
Electronic Supplementary Material (ESI) for Dalton Transactions.

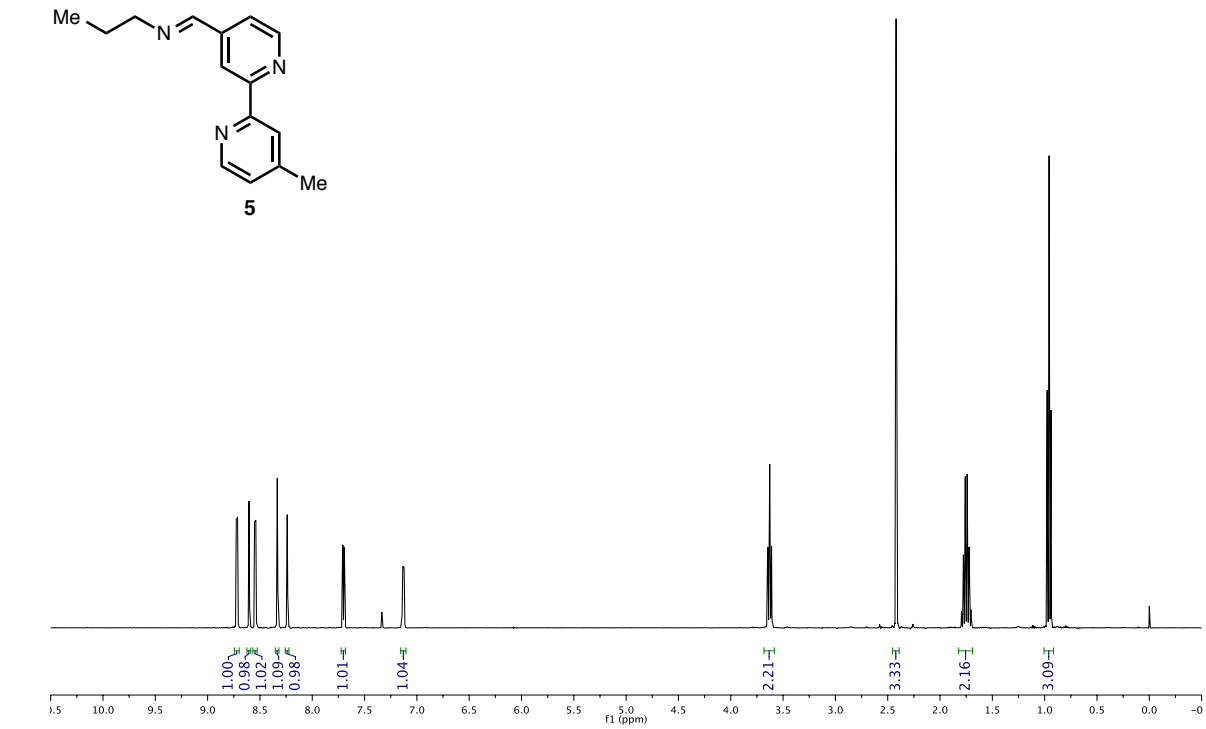
Influence of PNIPAm on log K_f of a copolymerized 2,2'-bipyridine: revised bifunctional ligand for ratiometric metal-ion sensing

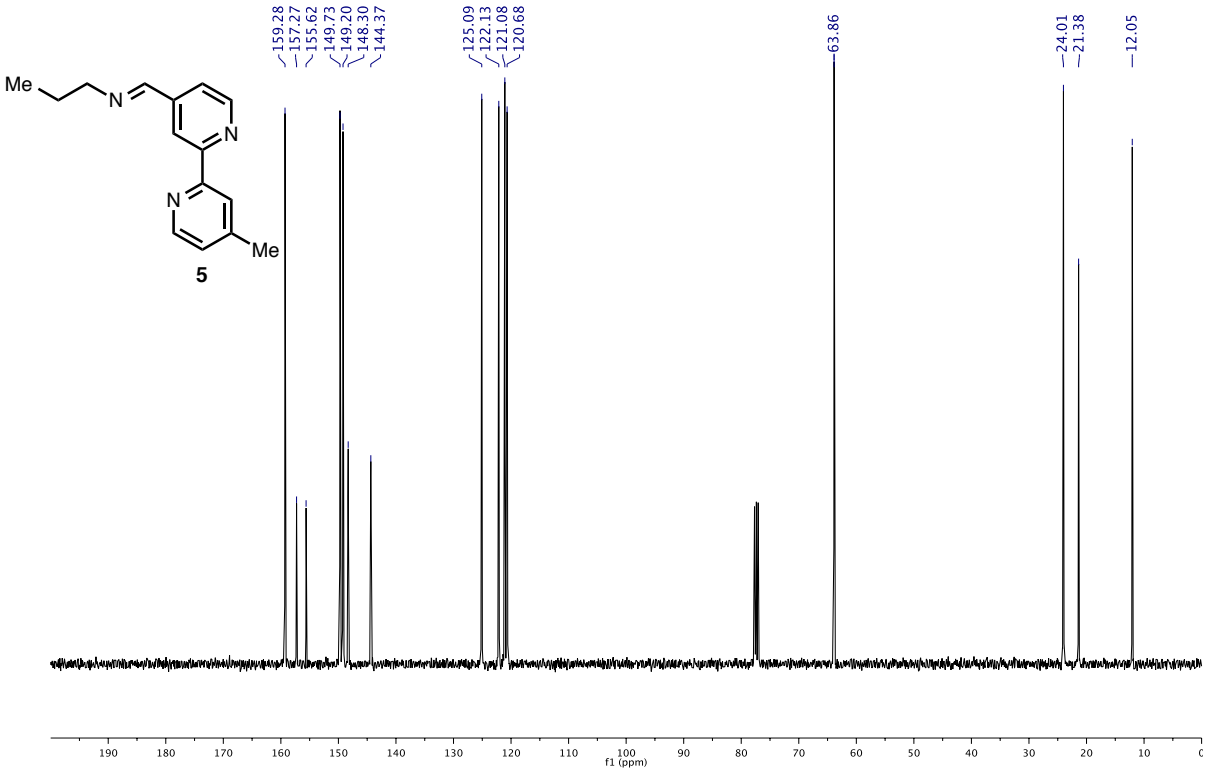
Justin O. Massing and Roy P. Planalp
Department of Chemistry, University of New Hampshire
Durham, NH 03824, United States

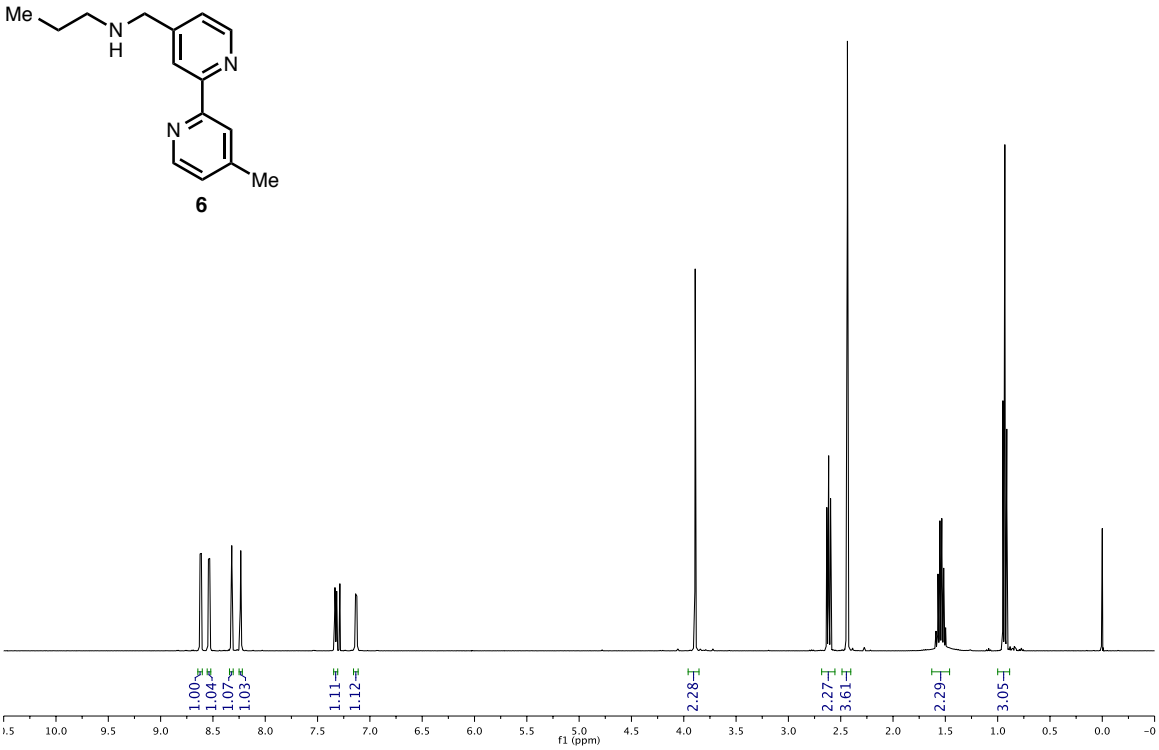
Supplementary Information

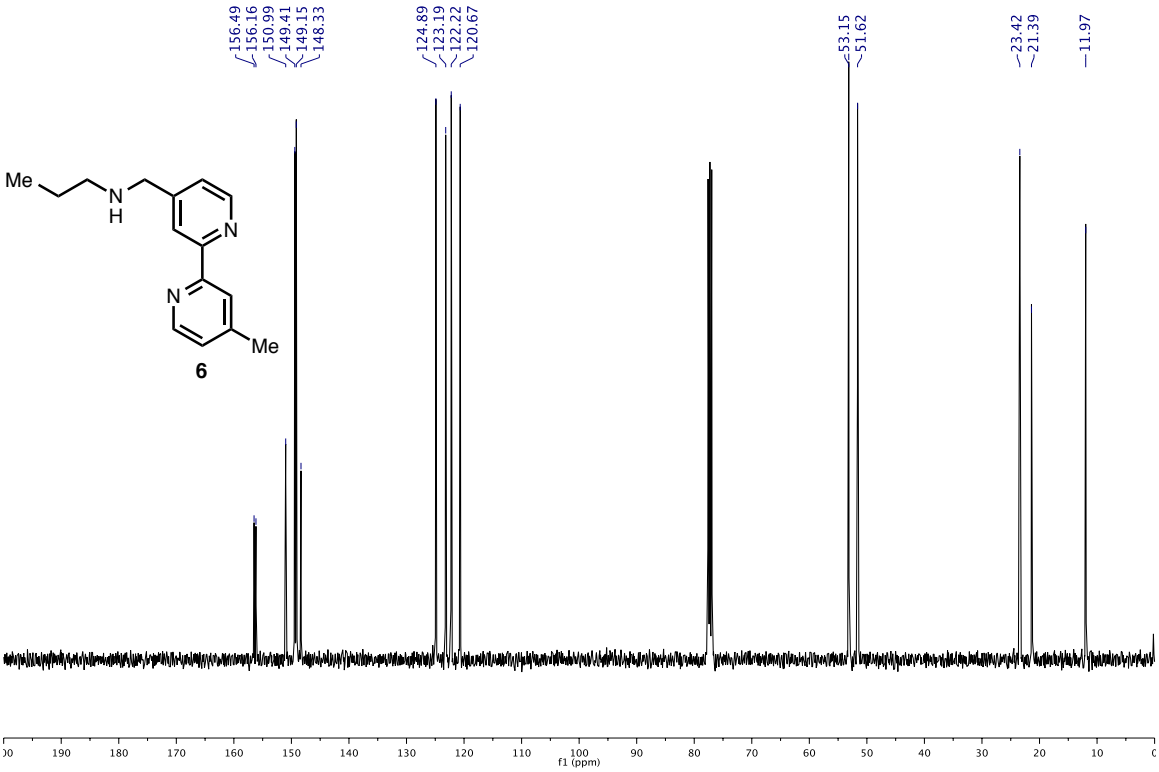

OHC
N
N
Me
4
1.00
0.93
1.01
0.95
0.98
1.00
1.03
3.32
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

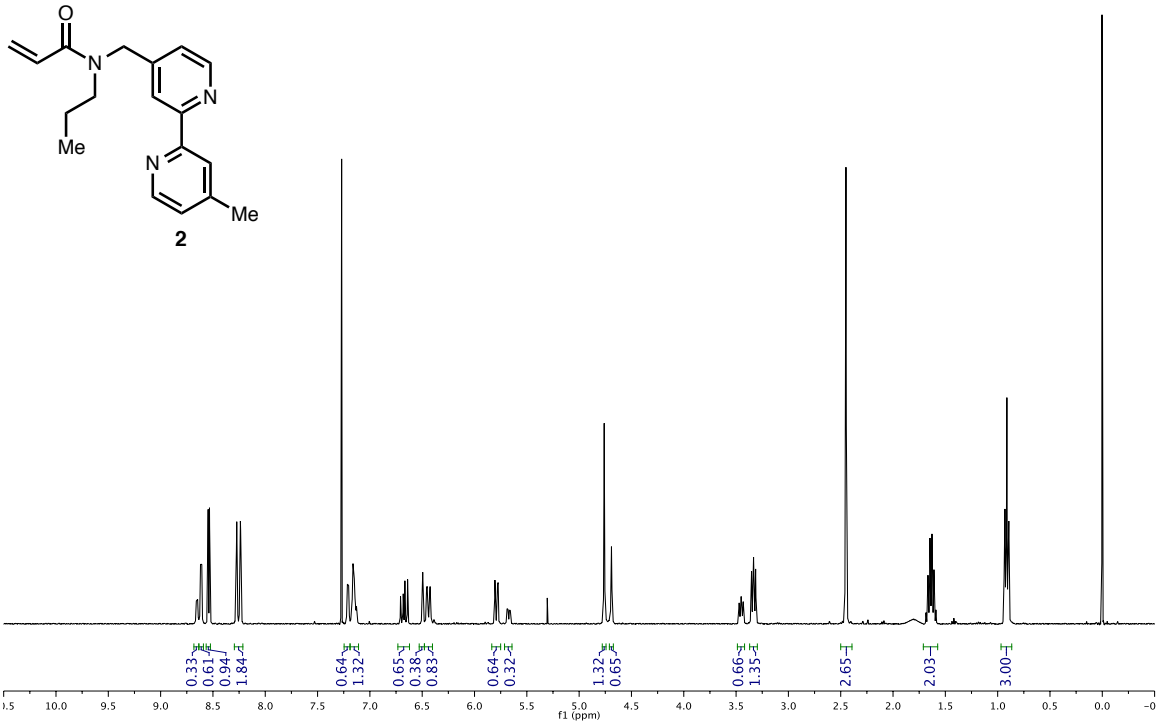

192.00
158.52
154.93
150.52
149.42
148.64
142.85
125.62
122.30
121.60
120.79
21.46
OHC
N
N
Me
4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

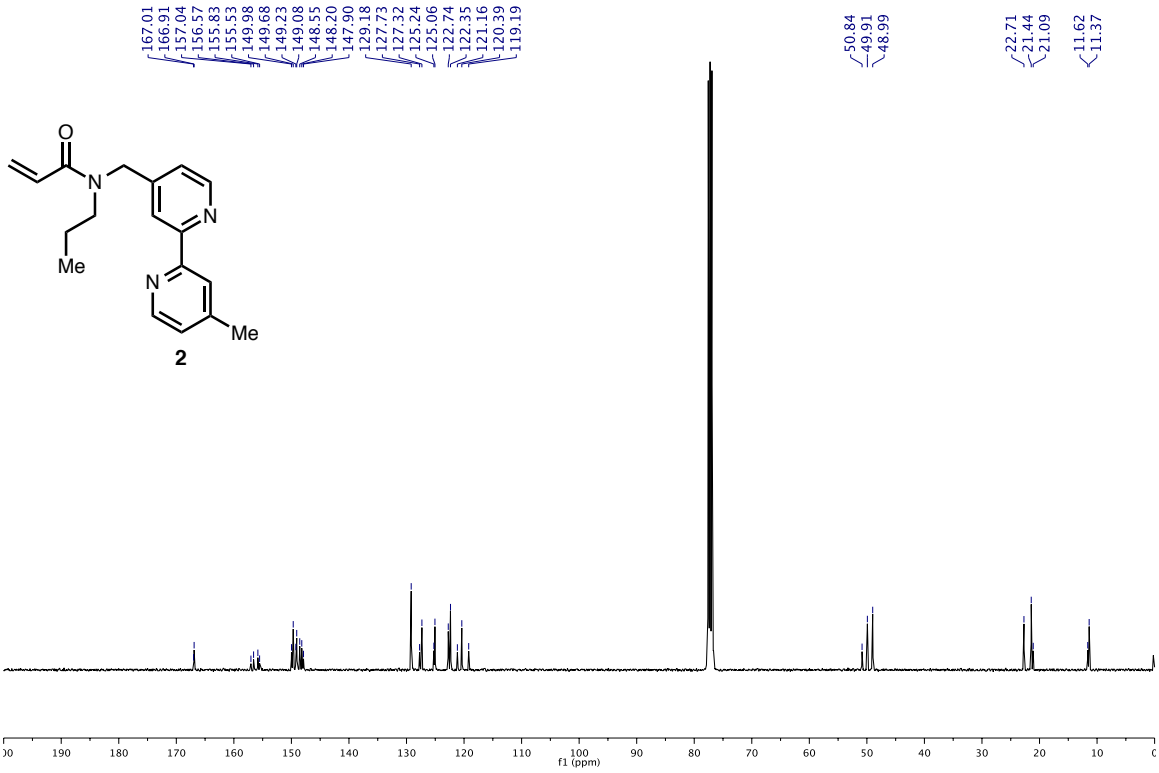

Me
N
N
N
Me
5
1.00
0.98
1.02
1.09
0.98
1.01
1.04
2.21
3.33
2.16
3.09
f1 (ppm)

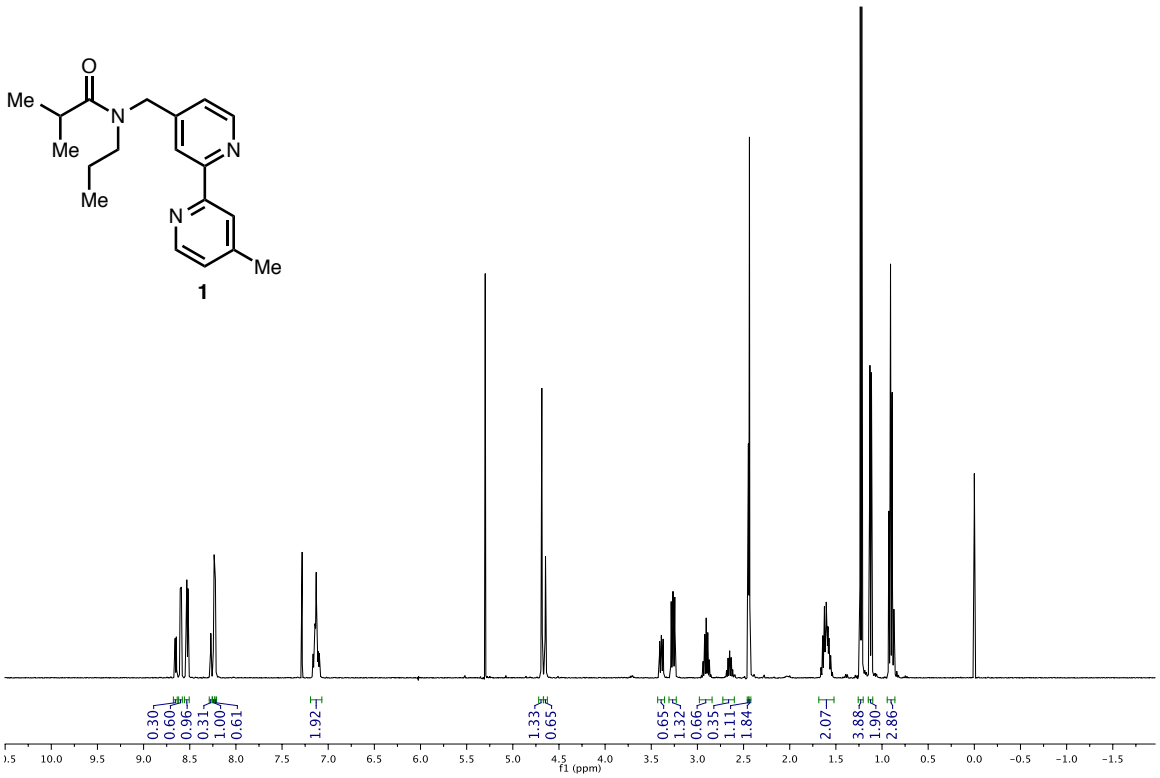

159.28
157.27
155.62
149.73
149.20
148.30
144.37
125.09
122.13
121.08
120.68
63.86
24.01
21.38
12.05
Me
N
N
N
Me
5
f1 (ppm)

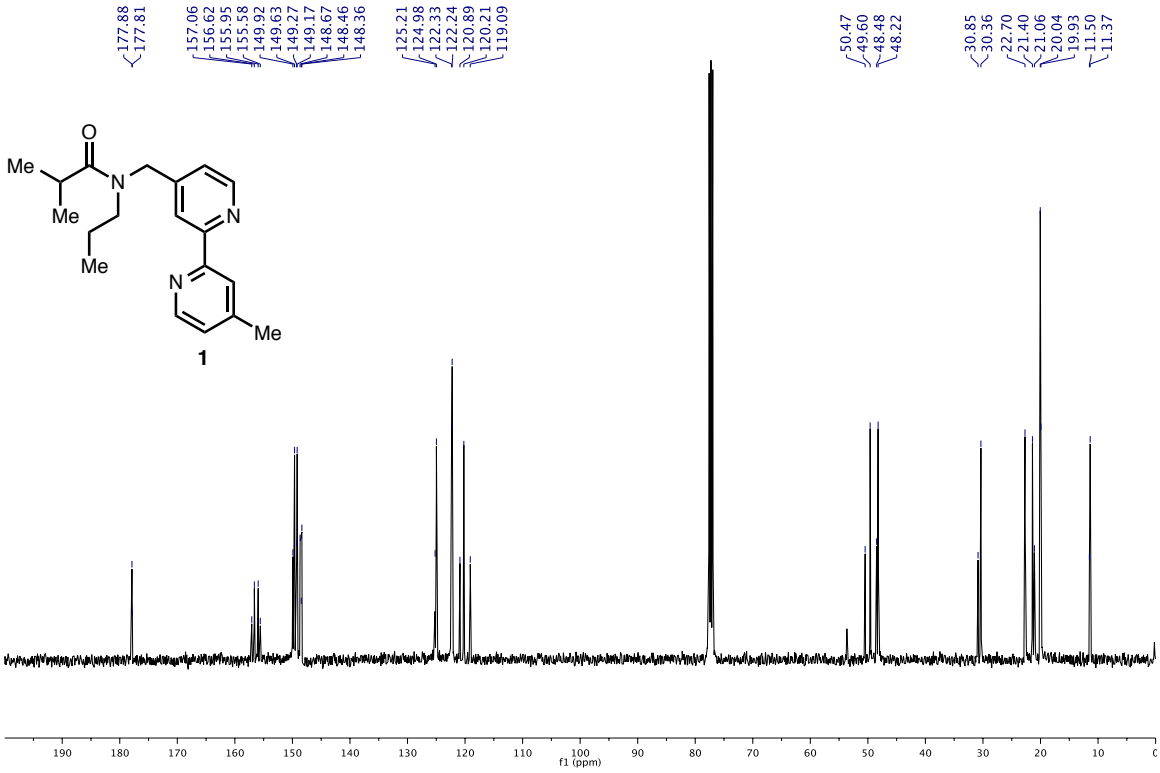

Me
N
H
N
N
Me
6
1.00
1.04
1.07
1.03
1.11
1.12
2.28
2.27
3.61
2.29
3.05
f1 (ppm)


156.49
156.16
150.99
149.41
149.15
148.33
124.89
123.19
122.22
120.67
53.15
51.62
23.42
21.39
11.97
Me
N
H
N
N
Me
6
f1 (ppm)


O
N
Me
N
N
Me
2
0.33
0.61
0.94
1.84
0.64
1.32
0.65
0.38
0.83
0.64
0.32
1.32
0.65
0.66
1.35
2.65
2.03
3.00
f1 (ppm)


167.01
166.91
157.04
156.57
155.83
155.53
149.98
149.68
149.23
149.08
148.55
148.20
147.90
129.18
127.73
127.32
125.24
125.06
122.74
122.35
121.16
120.39
119.19
50.84
49.91
48.99
22.71
21.44
21.09
11.62
11.37
O
N
Me
N
N
Me
2
f1 (ppm)


Me
Me
Me
O
N
N
N
Me
1
0.30
0.60
0.96
0.31
1.00
0.61
1.92
1.33
0.65
0.65
1.32
0.66
0.35
1.11
1.84
2.07
3.88
1.90
2.86
f1 (ppm)


177.88
177.81
157.06
156.62
155.95
155.58
149.92
149.63
149.27
149.17
148.67
148.46
148.36
125.21
124.98
122.33
122.24
120.89
120.21
119.09
50.47
49.60
48.48
48.22
30.85
30.36
22.70
21.40
21.06
20.04
19.93
11.50
11.37
Me
Me
Me
O
N
N
N
Me
1
f1 (ppm)

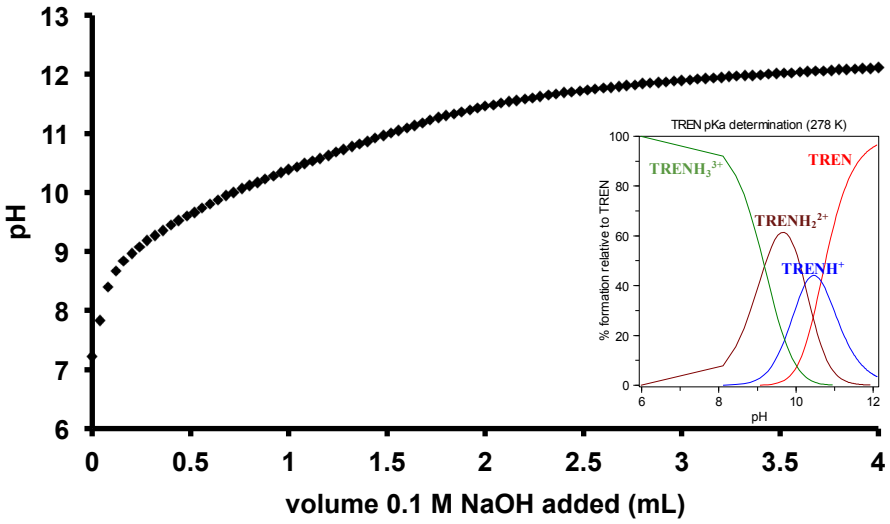


Figure S1. Potentiometric titration of 1.0 mM TREN·3HCl with NaOH at 5 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

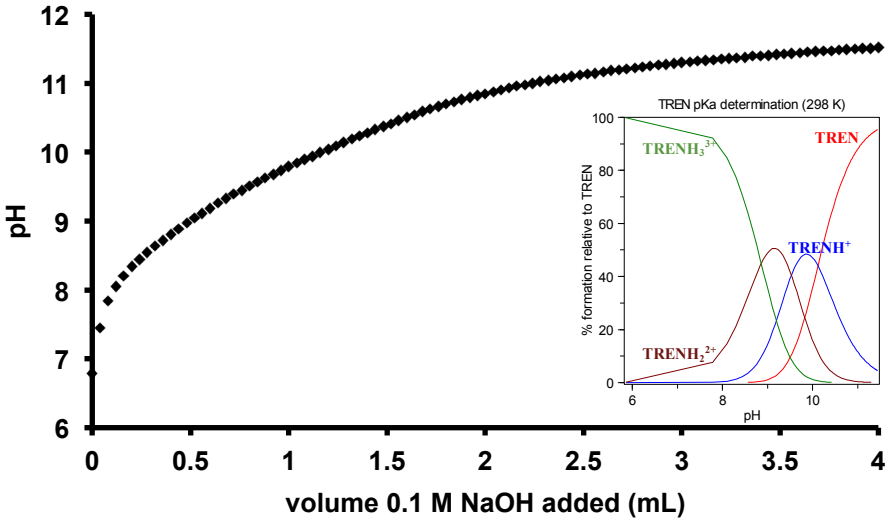


Figure S2. Potentiometric titration of 1.0 mM TREN·3HCl with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

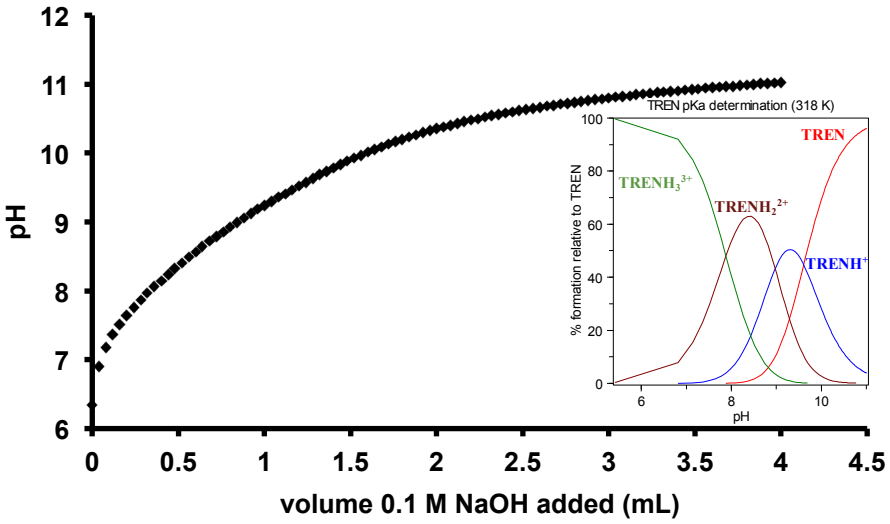


Figure S3. Potentiometric titration of 1.0 mM TREN·3HCl with NaOH at 45 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

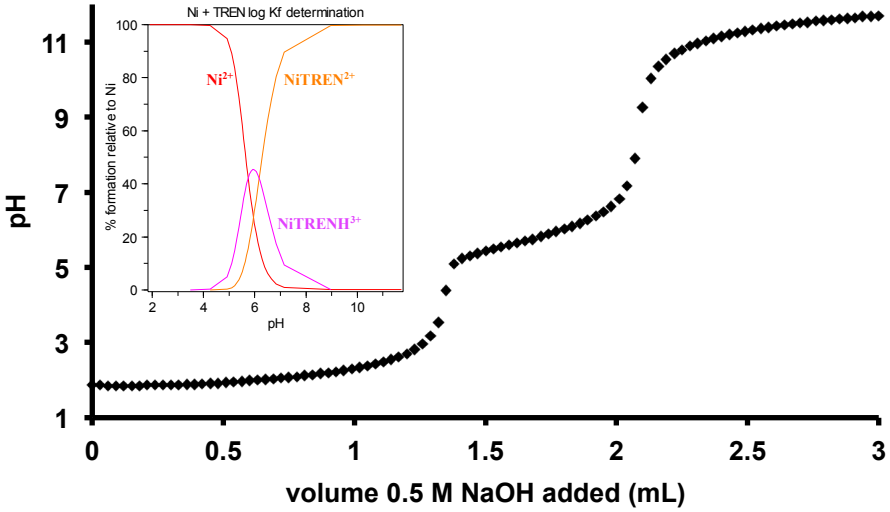


Figure S4. Potentiometric titration of 12.7 mM HNO_3 and equimolar (2.4 mM) TREN·3HCl and $Ni(NO_3)_2·6H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

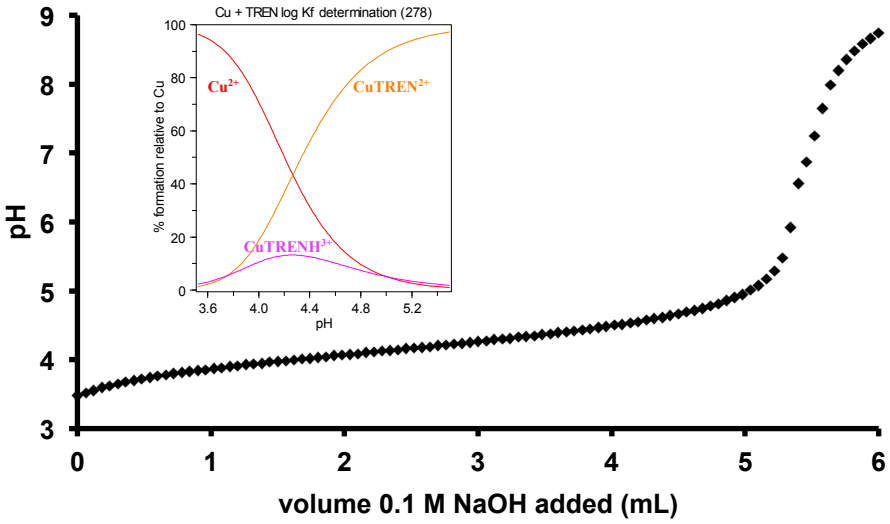


Figure S5. Potentiometric titration of equimolar (3.6 mM) TREN·3HCl and $Cu(NO_3)_2 \cdot 3H_2O$ with NaOH at 5 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

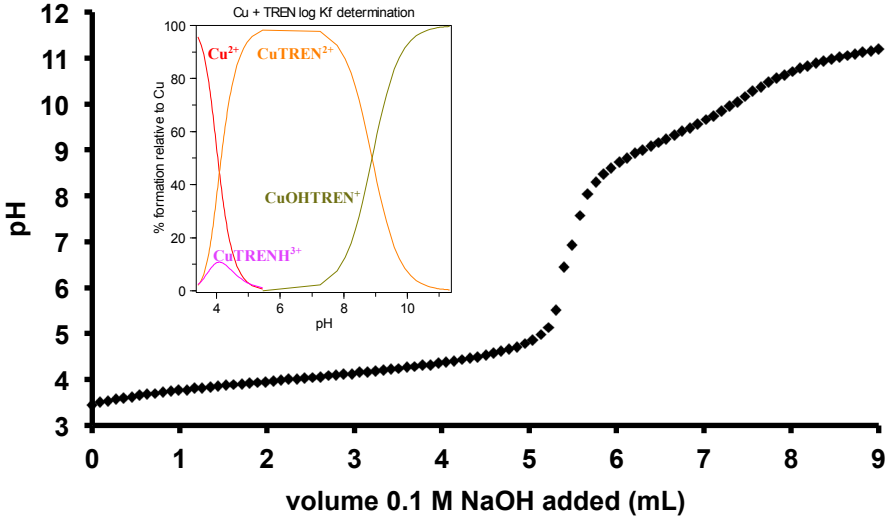


Figure S6. Potentiometric titration of equimolar (3.6 mM) TREN·3HCl and $Cu(NO_3)_2 \cdot 3H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

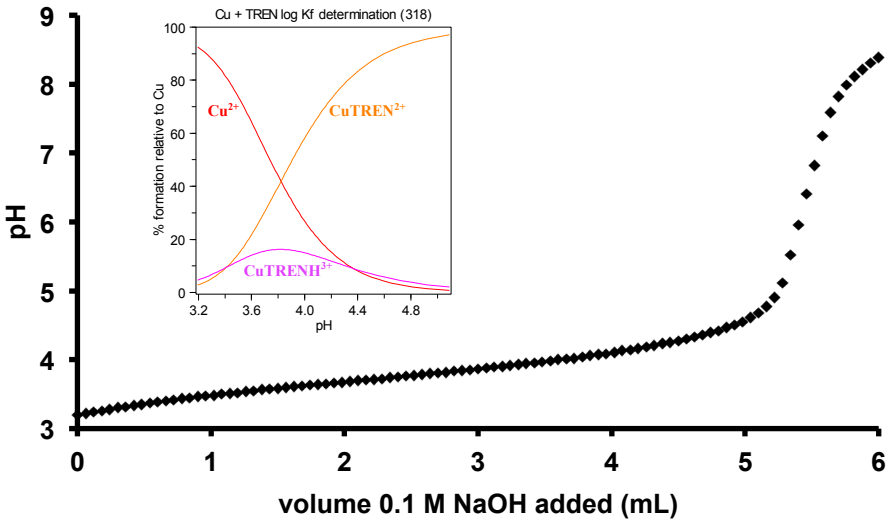


Figure S7. Potentiometric titration of equimolar (3.6 mM) TREN·3HCl and $Cu(NO_3)_2 \cdot 3H_2O$ with NaOH at 45 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

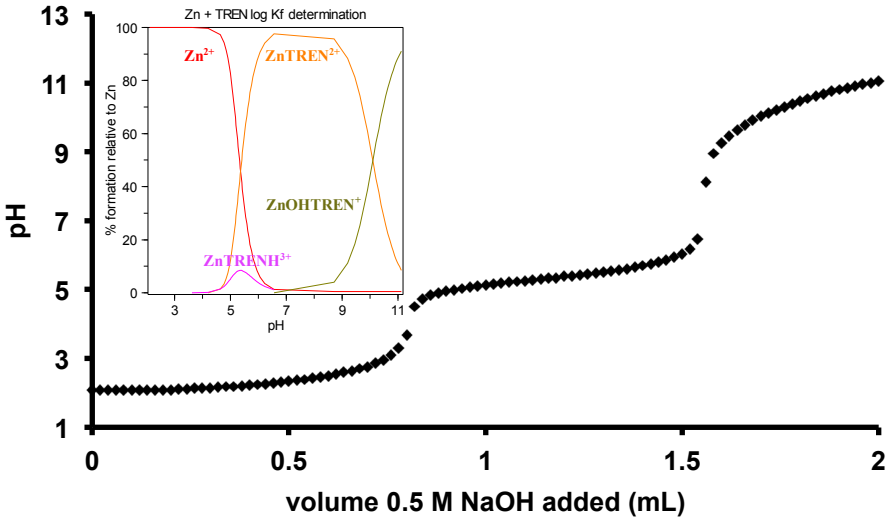


Figure S8. Potentiometric titration of 7.7 mM HNO_3 and equimolar (2.4 mM) TREN·3HCl and $Zn(NO_3)_2 \cdot 6H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

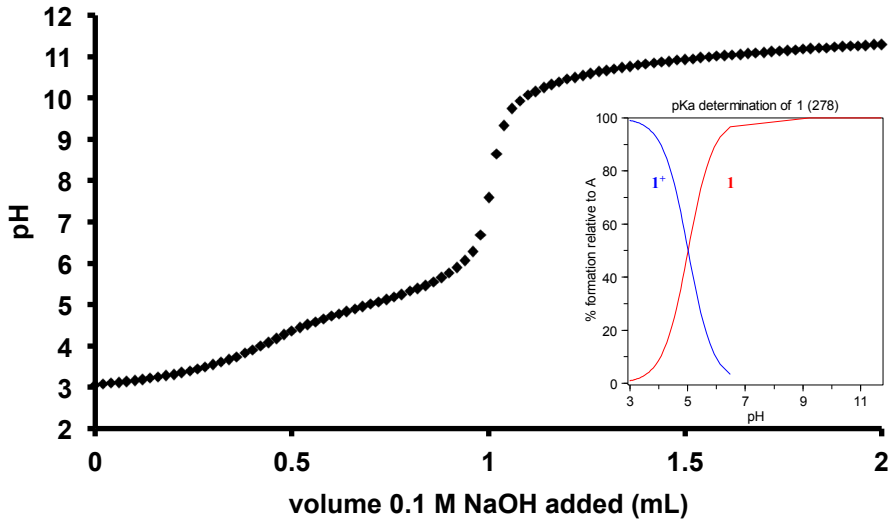


Figure S9. Potentiometric titration of 1.0 mM **1** and two equivalents of HNO_3 with NaOH at 5 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

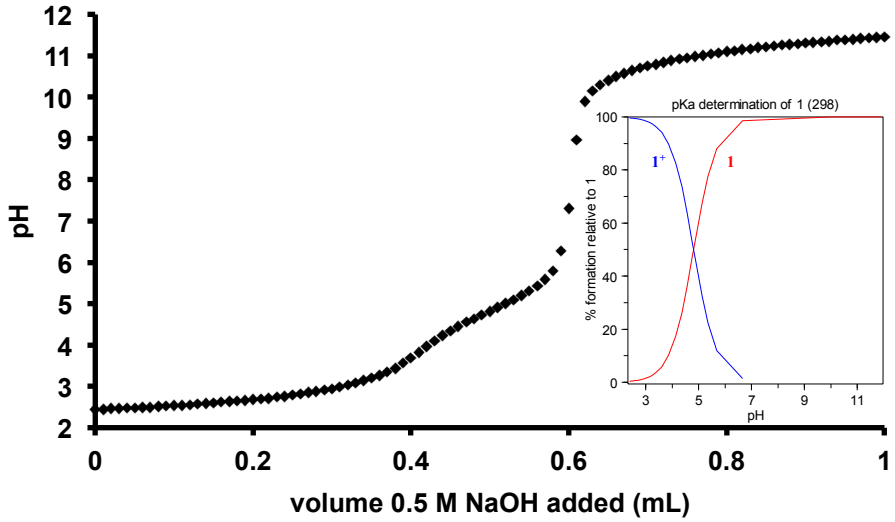


Figure S10. Potentiometric titration of 1.9 mM **1** and three equivalents of HNO_3 with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

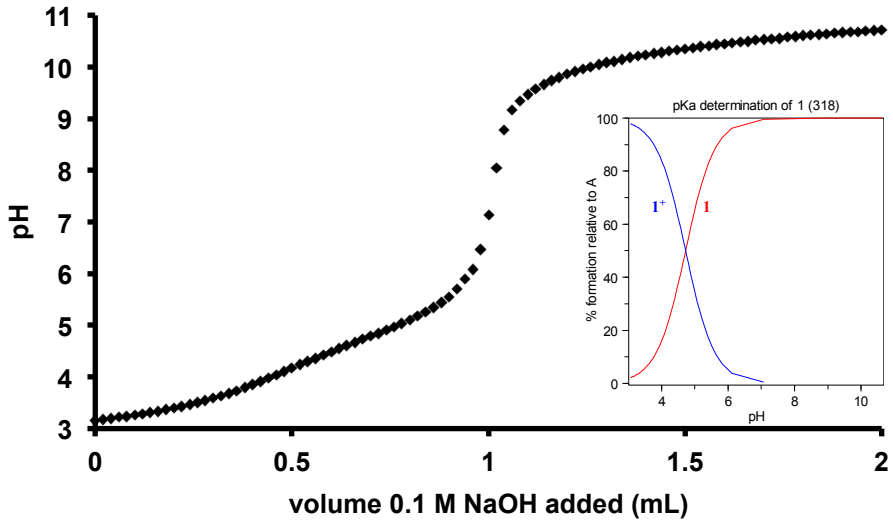


Figure S11. Potentiometric titration of 1.0 mM **1** and two equivalents of HNO_3 with NaOH at 45 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

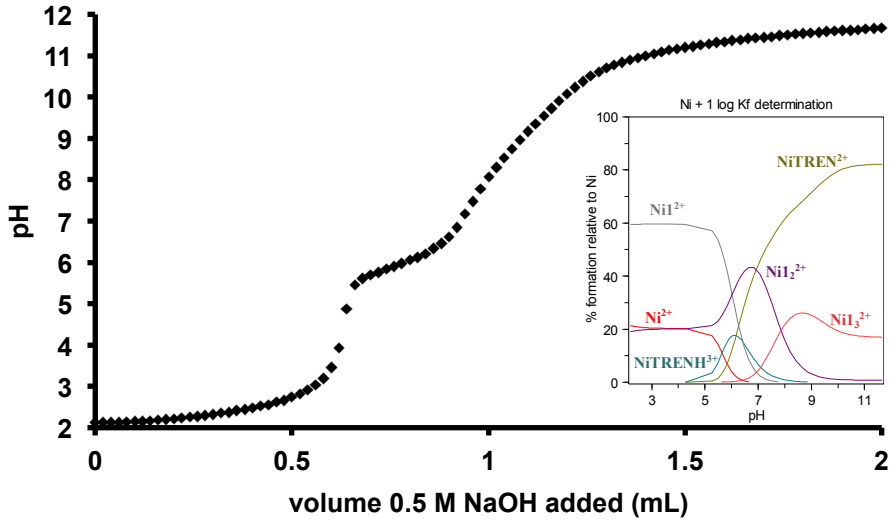


Figure S12. Potentiometric titration of equimolar (1.8 mM) **1**, TREN·3HCl, and $Ni(NO_3)_2{\cdot}6H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

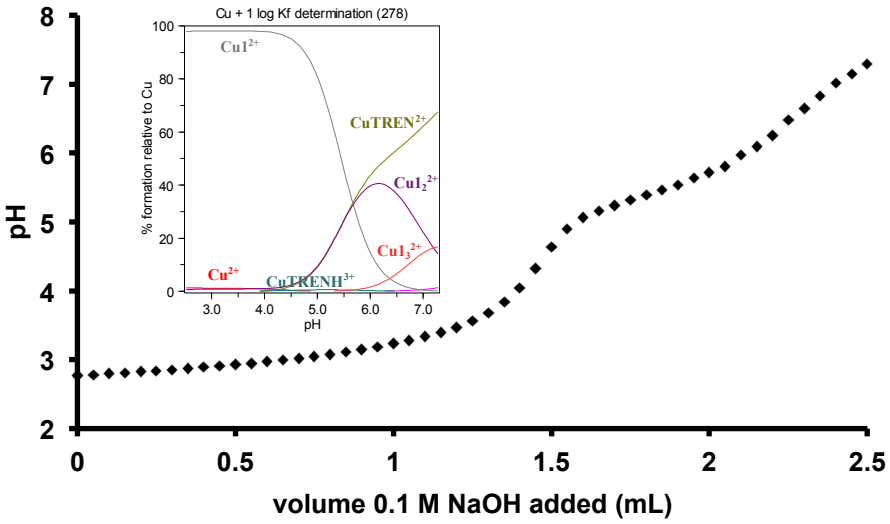


Figure S13. Potentiometric titration of equimolar (1.0 mM) **1**, TREN·3HCl, and $Cu(NO_3)_2 \cdot 3H_2O$ with NaOH at 5 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

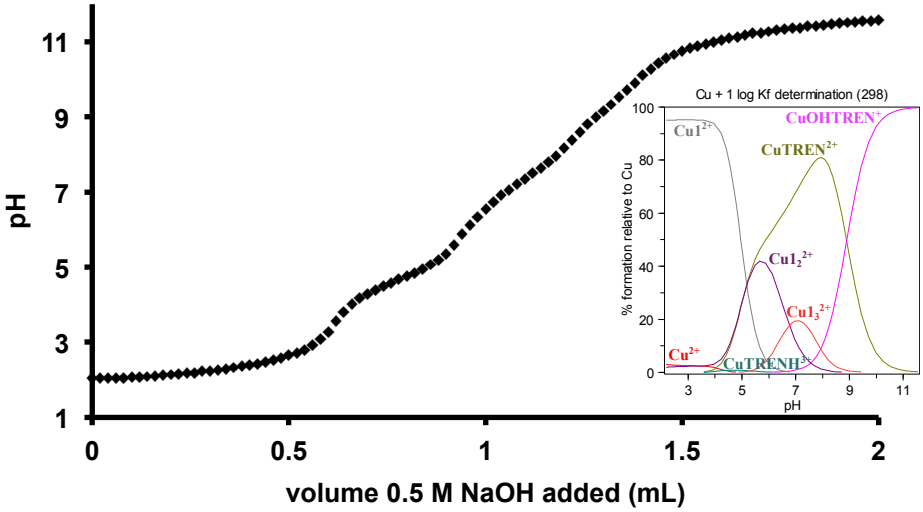


Figure S14. Potentiometric titration of equimolar (1.8 mM) **1**, TREN·3HCl, and $Cu(NO_3)_2 \cdot 3H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

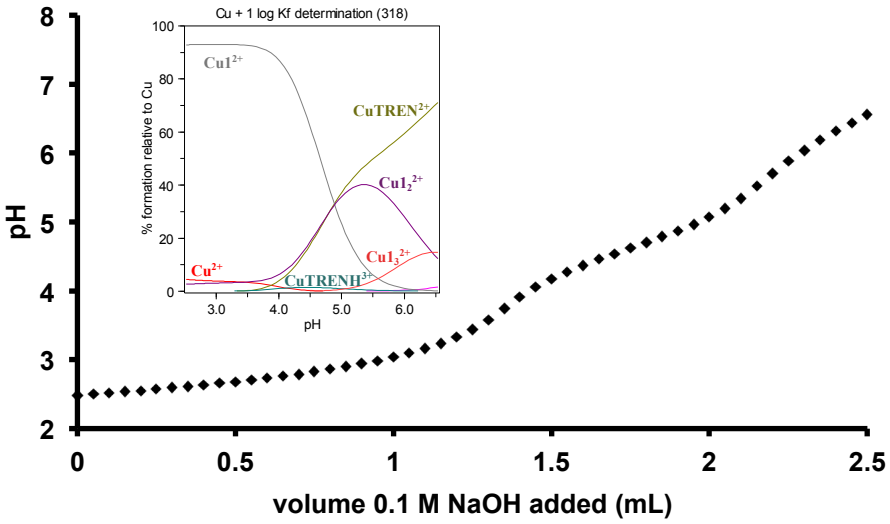


Figure S15. Potentiometric titration of equimolar (1.0 mM) **1**, TREN·3HCl, and $Cu(NO_3)_2{\cdot}3H_2O$ with NaOH at 45 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

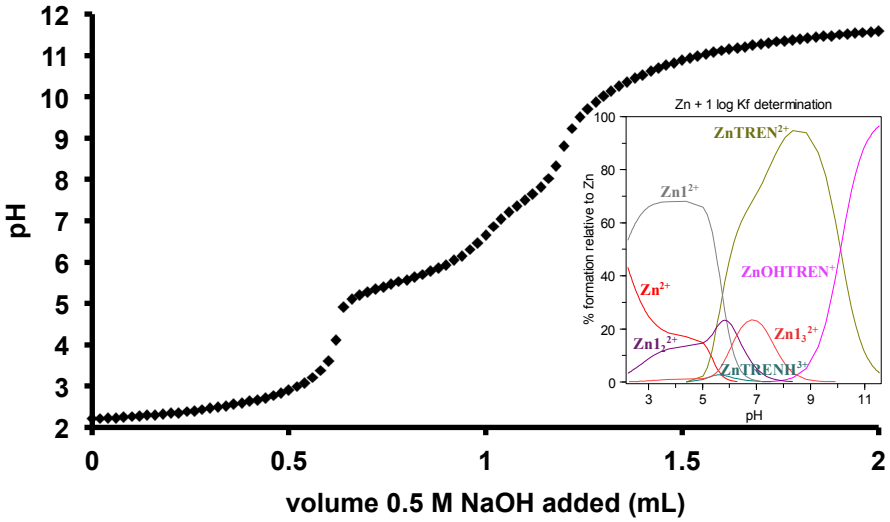


Figure S16. Potentiometric titration of equimolar (1.8 mM) **1**, TREN·3HCl, and $Zn(NO_3)_2{\cdot}6H_2O$ with NaOH at 25 ºC in 0.1 M $NaNO_3$. Corresponding distribution diagram (inset).

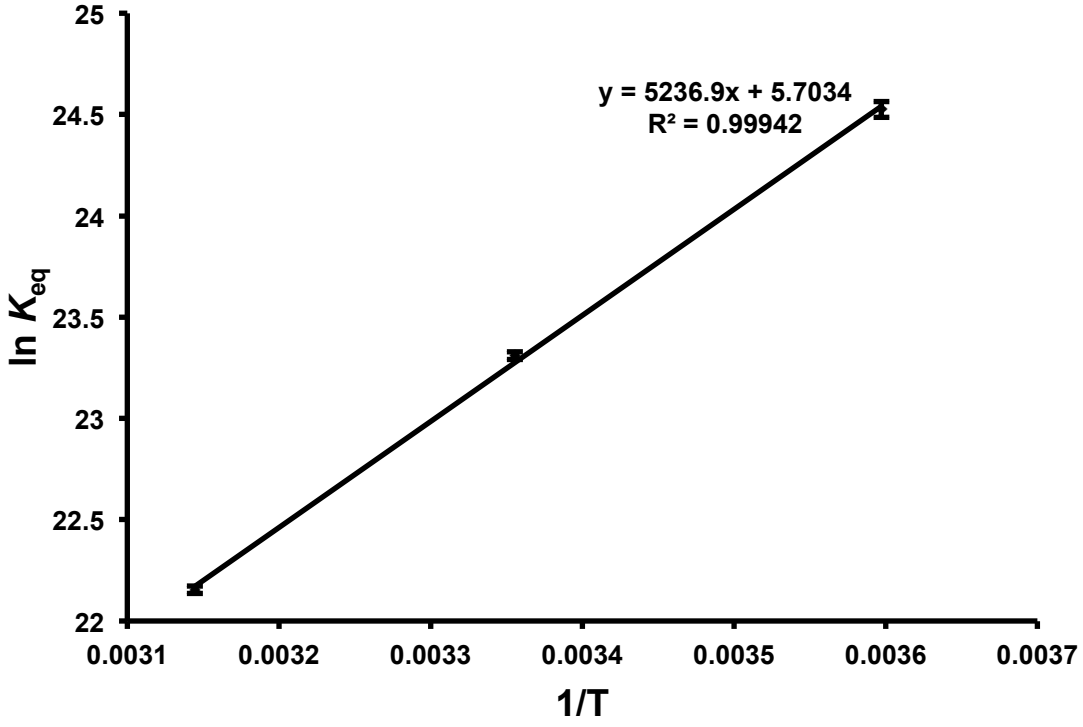


Figure S17. Van 't Hoff plot for $TRENH^{+}$.

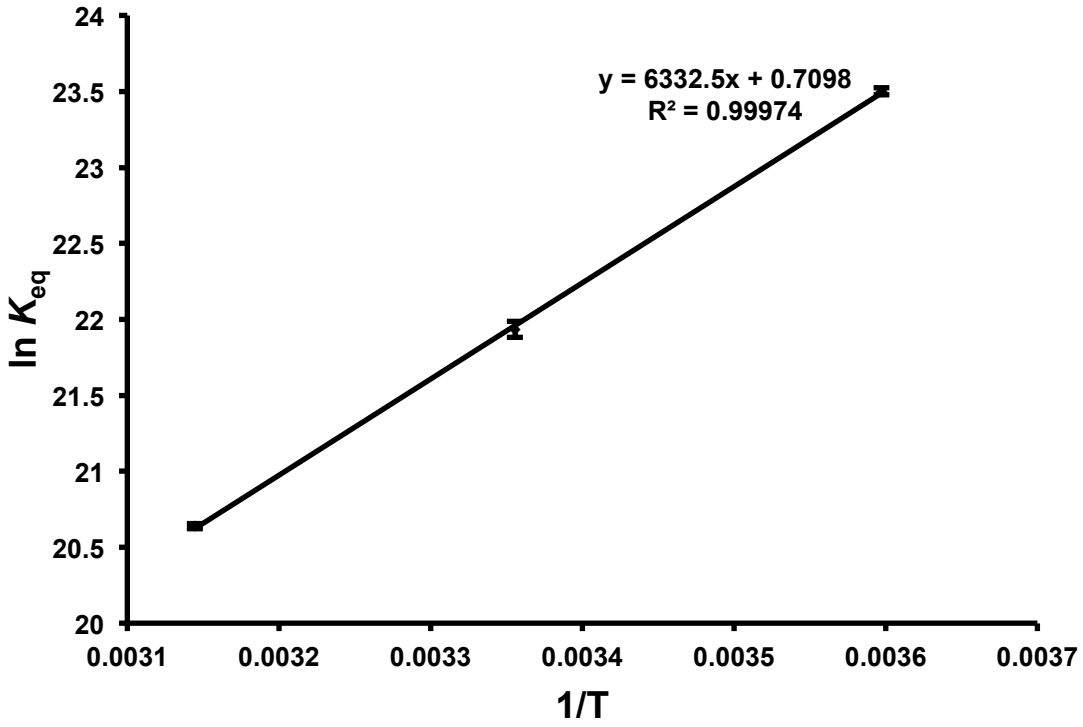


Figure S18. Van 't Hoff plot for $TRENH_2^{2+}$.

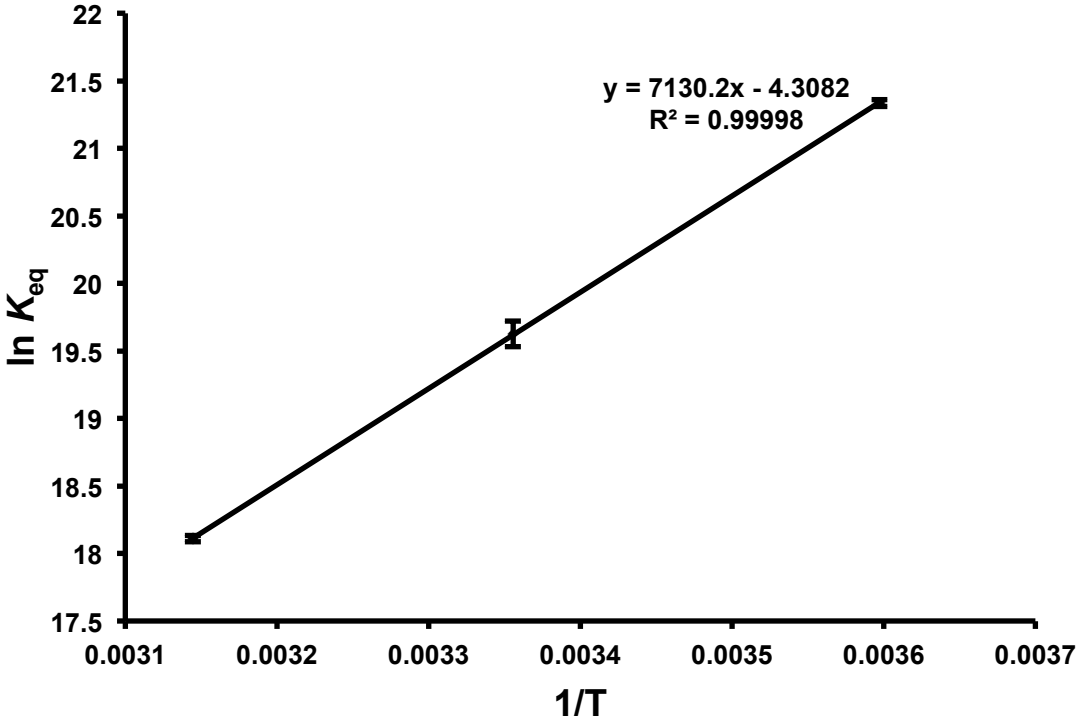


Figure S19. Van 't Hoff plot for $TRENH_3^{3+}$.

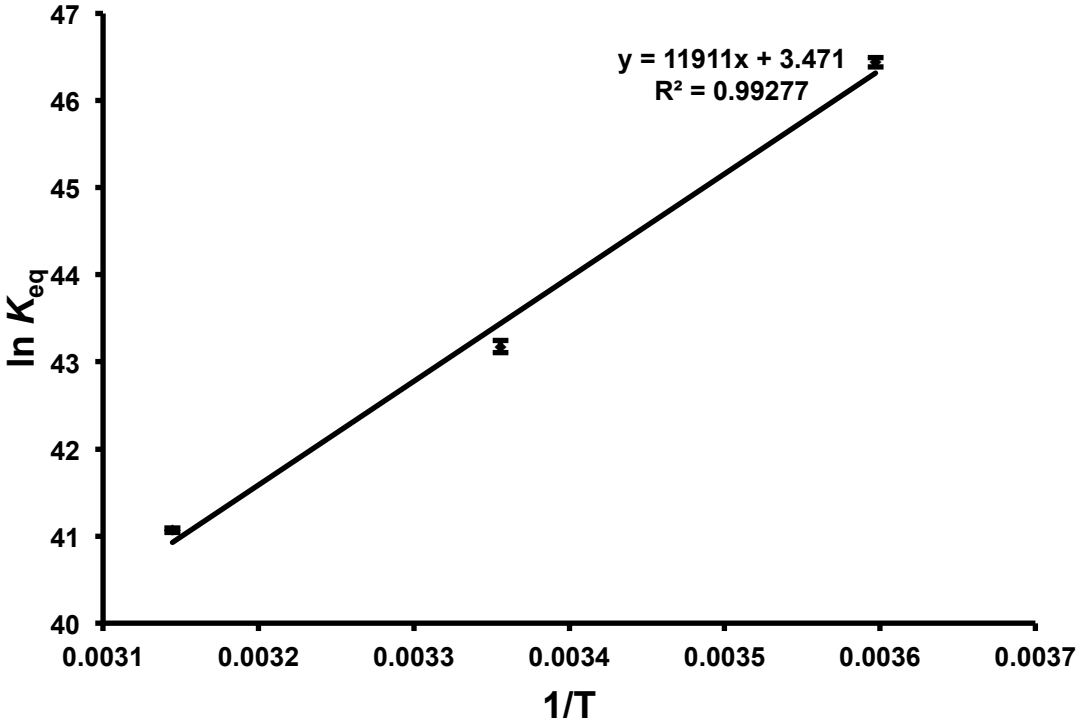


Figure S20. Van 't Hoff plot for $CuTREN^{2+}$.

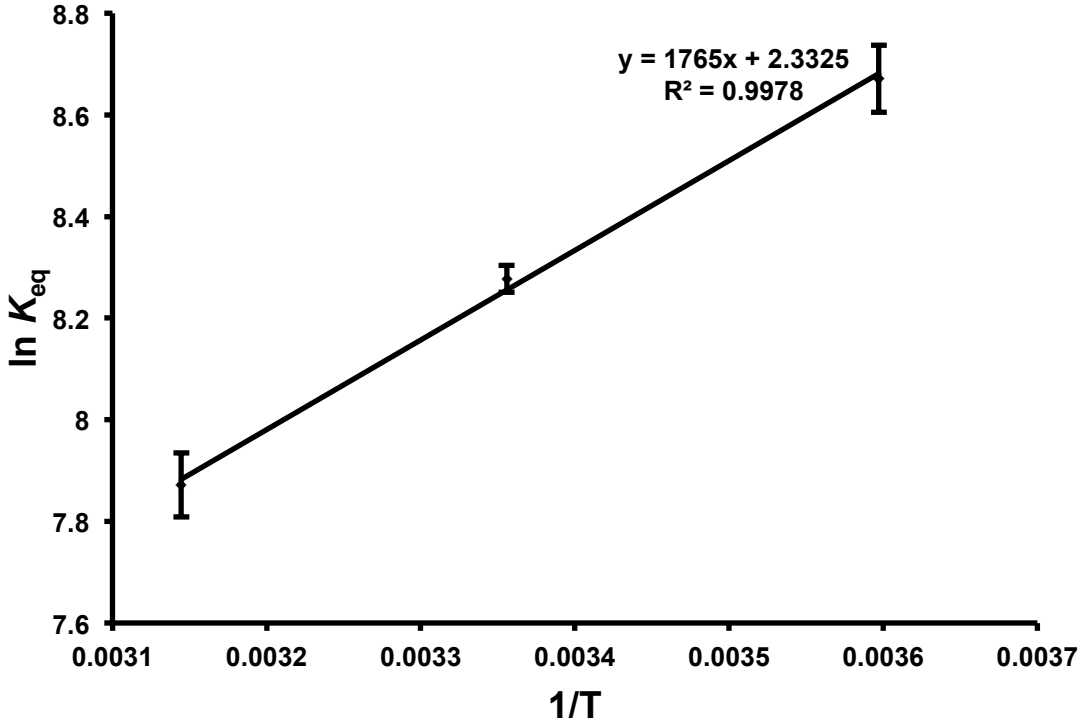


Figure S21. Van 't Hoff plot for $CuTRENH^{3+}$.

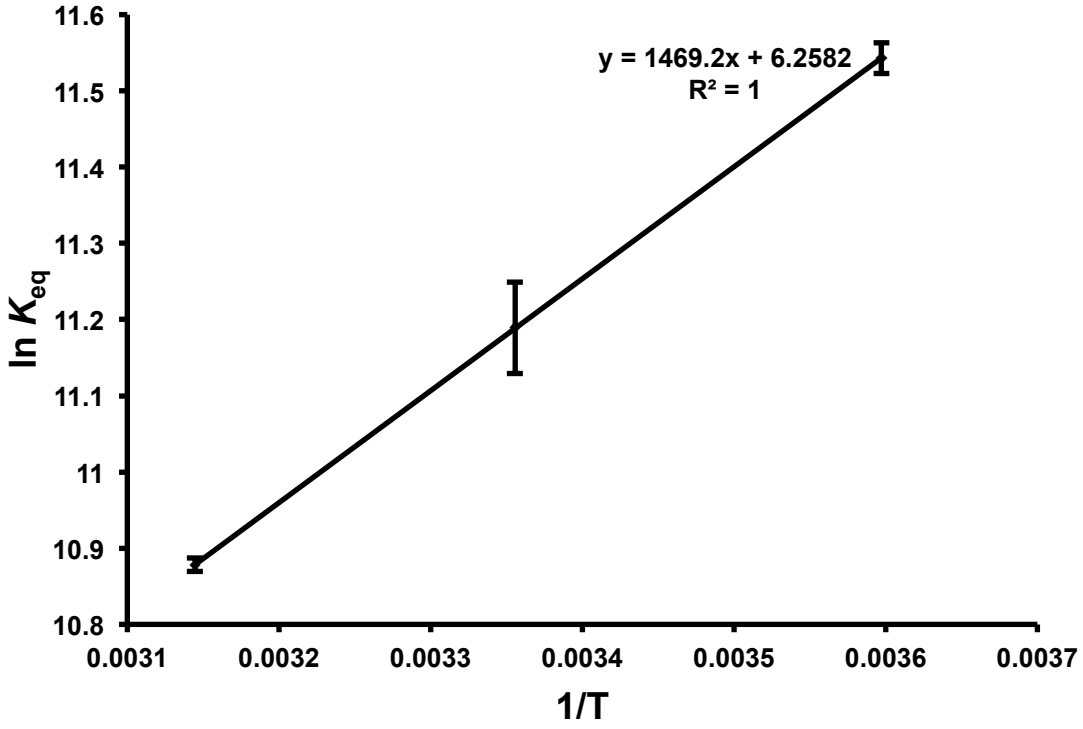


Figure S22. Van 't Hoff plot for **1**H^{+}.

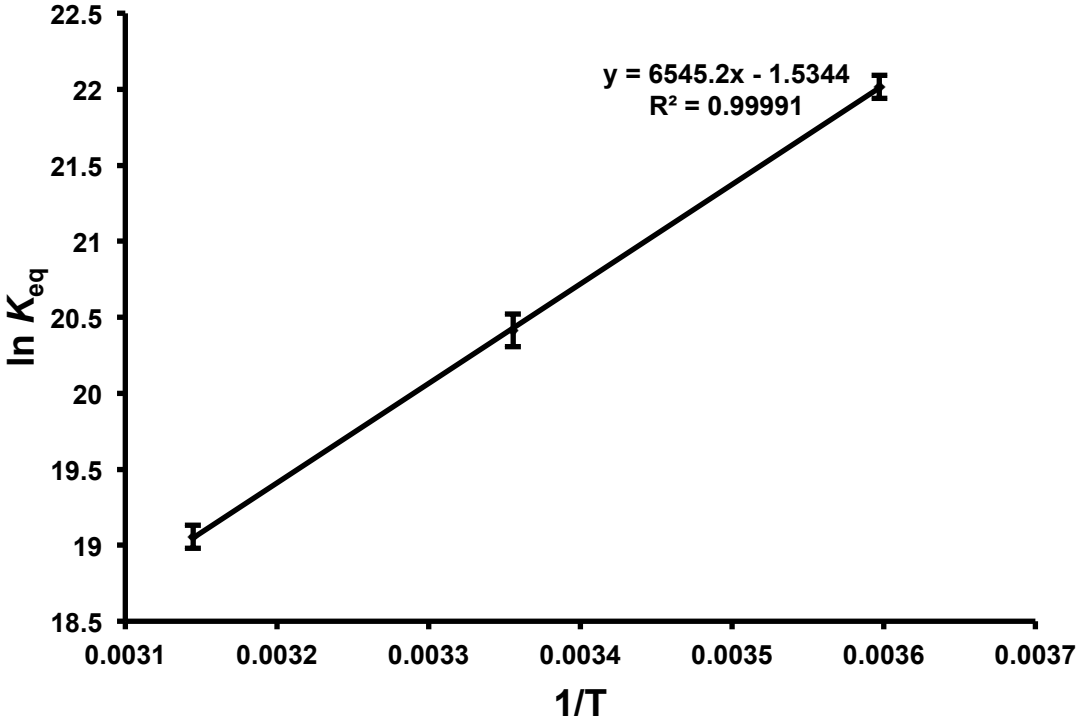


Figure S23. Van 't Hoff plot for Cu**1**$^{2+}$.