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Ligand design using the neutral oxygen donor to control metal ion size selectivity

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TITRANT H+ /M = 0.05019

V/ML	E/MV	PH	NBAR	TH	TH-NBAR
0.20	-220.4	9.34	0.07	0.09	0.01
0.40	-205.3	9.08	0.14	0.15	0.01
0.60	-194.9	8.90	0.21	0.22	0.01
0.80	-186.8	8.77	0.28	0.29	0.01
1.00	-180.3	8.66	0.35	0.35	0.01
1.20	-174.9	8.57	0.41	0.42	0.00
1.40	-169.2	8.47	0.48	0.49	0.01
1.60	-164.4	8.39	0.55	0.56	0.01
1.80	-160.0	8.31	0.62	0.63	0.01
2.00	-155.7	8.24	0.69	0.70	0.01
2.20	-151.9	8.18	0.76	0.77	0.01
2.40	-148.1	8.11	0.83	0.83	0.01
2.60	-144.4	8.05	0.90	0.90	0.00
2.80	-140.9	7.99	0.97	0.97	0.00
3.00	-136.8	7.92	1.04	1.04	0.01
3.20	-131.1	7.83	1.10	1.15	0.04
3.40	-129.6	7.80	1.17	1.17	0.00
3.60	-125.0	7.72	1.24	1.25	0.01
3.80	-121.1	7.66	1.31	1.32	0.01
4.00	-117.0	7.59	1.38	1.39	0.01
4.20	-112.3	7.51	1.45	1.46	0.01
4.40	-107.3	7.42	1.52	1.53	0.01
4.60	-101.5	7.33	1.59	1.60	0.02
4.80	-95.0	7.22	1.66	1.68	0.02
5.00	-86.7	7.08	1.72	1.75	0.03
5.20	-77.3	6.92	1.79	1.82	0.03
5.40	-65.5	6.72	1.86	1.88	0.02
5.60	-39.2	6.27	1.93	1.96	0.02
5.80	87.6	4.13	1.99	2.00	0.01
6.00	131.6	3.39	2.00	2.00	0.00
6.20	147.5	3.12	2.00	2.00	0.00
6.40	157.9	2.94	2.00	2.00	0.00
6.60	164.6	2.83	2.00	2.00	0.00

TITRATION 2

E0 /MV = 333.3
INIT VOL /ML = 20.00
LIG IN CELL/MMOL = 0.09860
TITRANT H+ /M = 0.05019

V/ML	E/MV	PH	NBAR	TH	TH-NBAR
0.20	-211.2	9.20	0.11	0.12	0.01
0.40	-195.4	8.94	0.21	0.21	0.00
0.60	-183.0	8.73	0.31	0.31	0.00
0.80	-174.3	8.59	0.41	0.40	-0.01
1.00	-166.7	8.45	0.51	0.51	0.00
1.20	-160.8	8.35	0.61	0.59	-0.02
1.40	-154.0	8.24	0.71	0.71	-0.01
1.60	-148.3	8.14	0.81	0.80	-0.01
1.80	-142.7	8.05	0.92	0.91	-0.01
2.00	-137.7	7.96	1.02	1.00	-0.02
2.20	-132.7	7.88	1.12	1.09	-0.03

PKA-DHP-15-aneN2O3

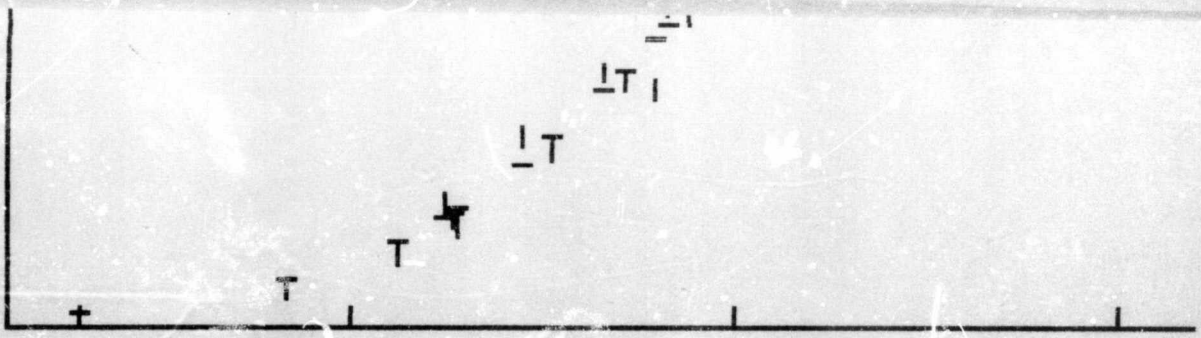
MATRIX CONDITION NUMBER = 1.0199
CONVERGENCE IN *2* CYCLES
RMSD = .0153
SUM DELTA SQUARED = .01

PARAMETERS AND ERRORS

LOG K (1) = 8.304 +- .007
LOG K (2) = 7.616 +- .007

TITRATION 1

E0 /MV = 331.9
INIT VOL /ML = 20.00
LIG IN CELL/MMOL = 0.14550



X - AXIS STARTS AT -9.9 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

| = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

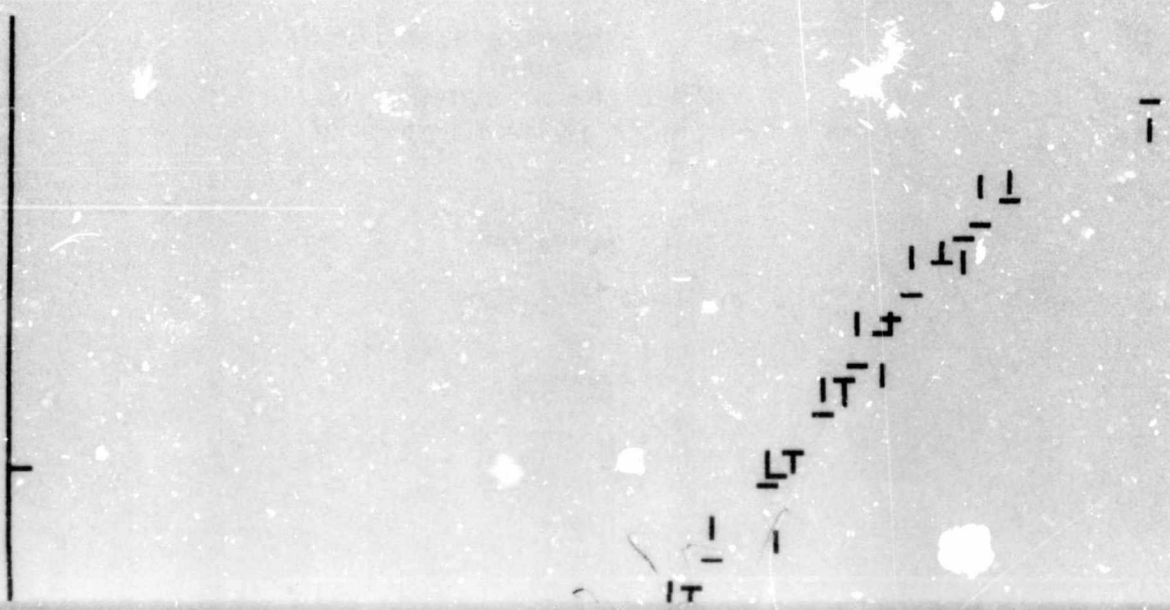
V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.10	78.9	-9.70	0.01	0.01	0.01
1.20	62.4	-9.16	0.04	0.05	0.01
1.30	53.4	-8.87	0.98	0.09	0.02
1.40	48.8	-8.73	0.12	0.12	0.01
1.60	40.3	-8.47	0.19	0.20	0.01
1.80	34.0	-8.29	0.27	0.28	0.01
2.00	28.0	-8.12	0.35	0.37	0.02
2.40	18.0	-7.85	0.50	0.51	0.01
2.60	12.8	-7.72	0.58	0.59	0.01
2.80	7.7	-7.59	0.66	0.66	0.00
3.00	2.4	-7.46	0.74	0.72	-0.01
3.20	-4.2	-7.29	0.81	0.80	-0.02

TITRATION 3

E0	/MV	=	332.1
INIT VOL.	/ML	=	20.00
H+ IN CELL	/MMOL	=	0.07530
LIG IN CELL	/MMOL	=	0.0290
M IN CELL.	/MMOL	=	0.01650
TITRANT B-	/M	=	0.05150

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
0.40	33.8	-8.71	0.11	0.13	0.02
0.50	17.3	-8.20	0.26	0.32	0.06
0.60	6.9	-7.90	0.42	0.49	0.07
0.72	-3.5	-7.62	0.60	0.65	0.05
0.80	-11.4	-7.40	0.72	0.75	0.03
0.90	-27.9	-6.92	0.87	0.90	0.03

Log K1(CuII)-DHP-15-ane-N2O3



Log K1(CuII)-DHP-15-ane-N2O3

ACID CONSTANTS:

PKA (1) = 8.30
PKA (2) = 7.62

MATRIX CONDITION NUMBER = 1.0000
CONVERGENCE IN *3* CYCLES
RMSD = .0305
SUM DELTA SQUARED = .03

PARAMETERS AND ERRORS

LOG K (1) = 7.879 +- .013

TITRATION 1

E0 /MV = 332.5
INIT VOL /ML = 19.00
LIG IN CELL/MMOL = 0.07395
M IN CELL /MMOL = 0.06660
TITRANT H+ /M = 0.05019

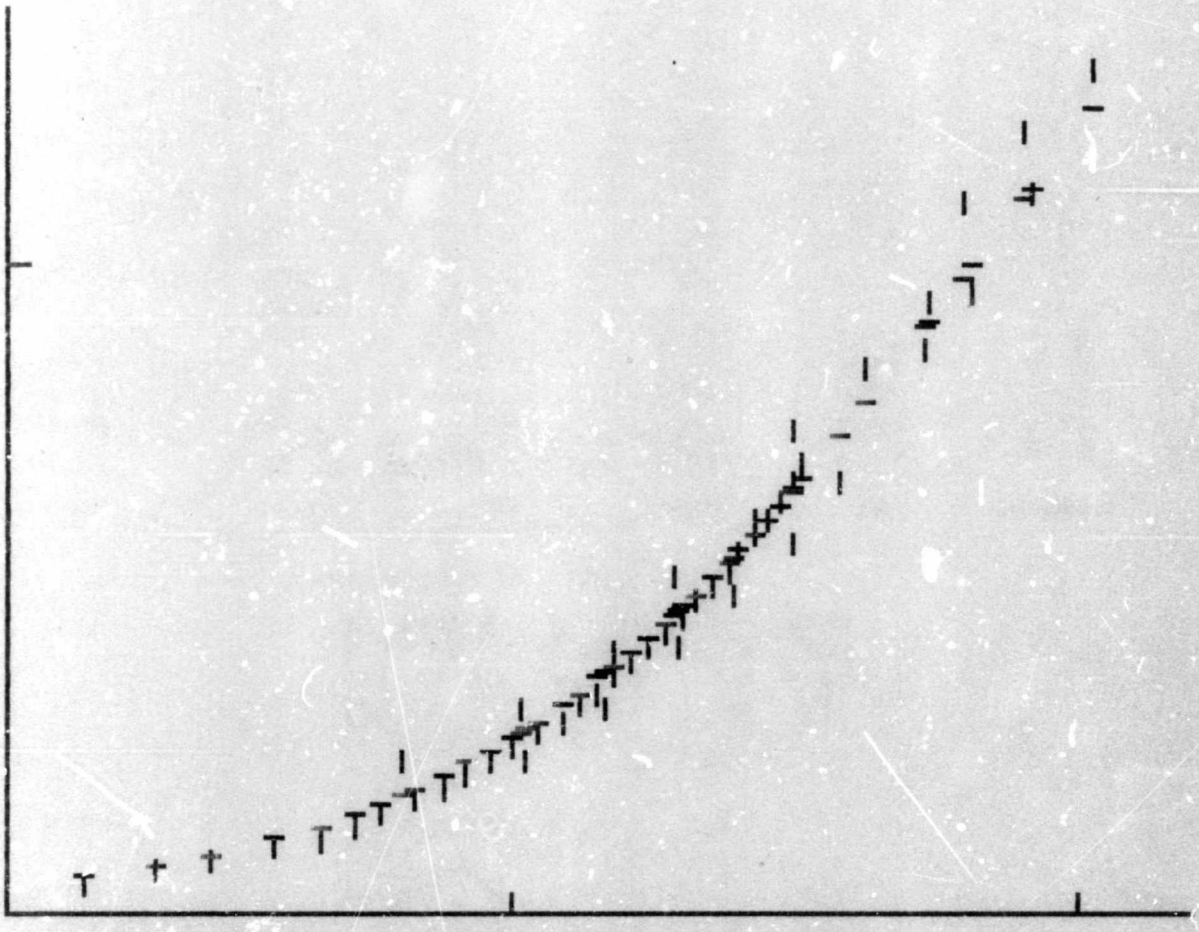
V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.00	-9.5	-7.36	0.81	0.77	-0.04
1.08	1.6	-7.53	0.73	0.69	-0.04
1.20	5.2	-7.69	0.66	0.61	-0.05
1.40	9.7	-7.78	0.58	0.56	-0.02
1.60	15.4	-7.92	0.51	0.48	-0.03
1.80	21.2	-8.06	0.43	0.39	-0.04
2.00	25.5	-8.17	0.36	0.34	-0.02
2.20	31.6	-8.34	0.28	0.26	-0.02
2.40	38.9	-8.55	0.21	0.18	-0.03
2.60	45.8	-8.75	0.13	0.12	-0.01

TITRATION 2

E0 /MV = 332.1
INIT VOL /ML = 20.00
H+ IN CELL/MMOL = 0.25100
LIG IN CELL/MMOL = 0.09700
M IN CELL /MMOL = 0.06600
TITRANT B- /M = 0.05150

4.20	-51.2	-3.53	0.32	0.31	0.00
4.30	-54.9	-3.50	0.33	0.33	-0.01
4.40	-58.9	-3.49	0.35	0.33	-0.01

Log K1(BaII)-DHP-15-aneN2O3



X - AXIS STARTS AT -4.9 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

| = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

E0 /MV = 332.4
INIT VOL /ML = 19.00
LIG IN CELL/MMOL = 0.07298
M IN CELL /MMOL = 0.06660
TITRANT H+ /M = 0.05019

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
0.20	-181.0	-2.97	0.65	0.62	-0.03
0.40	-160.4	-3.10	0.60	0.55	-0.05
0.60	-148.0	-3.21	0.55	0.49	-0.06
0.80	-140.5	-3.27	0.47	0.46	-0.01
1.00	-132.4	-3.38	0.42	0.39	-0.03
1.20	-125.0	-3.50	0.37	0.33	-0.04
1.40	-120.0	-3.58	0.30	0.29	-0.01
1.60	-113.2	-3.71	0.26	0.23	-0.03
1.80	-108.0	-3.82	0.20	0.19	-0.01
2.00	-101.0	-3.99	0.16	0.14	-0.02
2.20	-93.0	-4.20	0.12	0.09	-0.03

TITRATION 3

E0 /MV = 417.0
INIT VOL /ML = 20.00
H+ IN CELL/MMOL = 0.24900
LIG IN CELL/MMOL = 0.09700
M IN CELL /MMOL = 0.19980
TITRANT B- /M = 0.05090

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.50	15.0	-4.76	0.02	0.03	0.00
1.63	10.8	-4.64	0.03	0.03	0.00
1.70	7.2	-4.53	0.04	0.04	0.00
1.82	3.0	-4.42	0.05	0.06	0.01
1.99	0.1	-4.34	0.05	0.07	0.01
2.00	-2.3	-4.28	0.06	0.07	0.01
2.10	-4.2	-4.24	0.07	0.08	0.01
2.20	-6.7	-4.18	0.08	0.09	0.01
2.30	-9.0	-4.12	0.09	0.10	0.01
2.40	-11.0	-4.08	0.10	0.11	0.01
2.50	-13.0	-4.04	0.12	0.12	0.01
2.60	-15.0	-4.00	0.13	0.13	0.01
2.70	-17.0	-3.96	0.14	0.15	0.01
2.80	-19.2	-3.91	0.15	0.16	0.01
2.90	-21.0	-3.88	0.16	0.17	0.01
3.00	-23.0	-3.85	0.17	0.18	0.01
3.10	-24.9	-3.82	0.18	0.19	0.01
3.20	-26.8	-3.79	0.19	0.20	0.01
3.30	-28.8	-3.76	0.20	0.21	0.01
3.40	-30.8	-3.73	0.22	0.22	0.01
3.50	-33.0	-3.70	0.23	0.24	0.01
3.60	-35.0	-3.68	0.24	0.24	0.00
3.70	-37.5	-3.65	0.25	0.26	0.01
3.80	-39.9	-3.62	0.26	0.27	0.01
3.90	-42.3	-3.60	0.26	0.28	0.00
4.00	-45.0	-3.57	0.29	0.29	0.00
4.10	-48.0	-3.55	0.30	0.30	0.00

Log K1(BaII)-DHP-15-aneN203

ACID CONSTANTS:

PKA (1) = 8.30
PKA (2) = 7.62

MATRIX CONDITION NUMBER = 1.0000
CONVERGENCE IN *2* CYCLES
RMSD = .0209
SUM DELTA SQUARED = .02

PARAMETERS AND ERRORS

LOG K (1) = 3.188 +- .007

TITRATION 1

E0 /MV = 417.7
INIT VOL /ML = 20.00
H+ IN CELL/MMOL = 0.25100
LIG IN CELL/MMOL = 0.09700
M IN CELL /MMOL = 0.06660
TITRANT B- /M = 0.05150

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
2.00	-11.2	-3.98	0.12	0.14	0.02
2.20	-17.1	-3.83	0.16	0.18	0.03
2.42	-22.8	-3.70	0.20	0.23	0.03
2.60	-27.2	-3.61	0.24	0.27	0.03
2.80	-32.6	-3.50	0.28	0.33	0.04
3.00	-37.2	-3.42	0.33	0.37	0.04
3.40	-46.9	-3.27	0.44	0.45	0.02
3.60	-52.8	-3.19	0.48	0.50	0.02
3.90	-62.2	-3.08	0.55	0.56	0.01

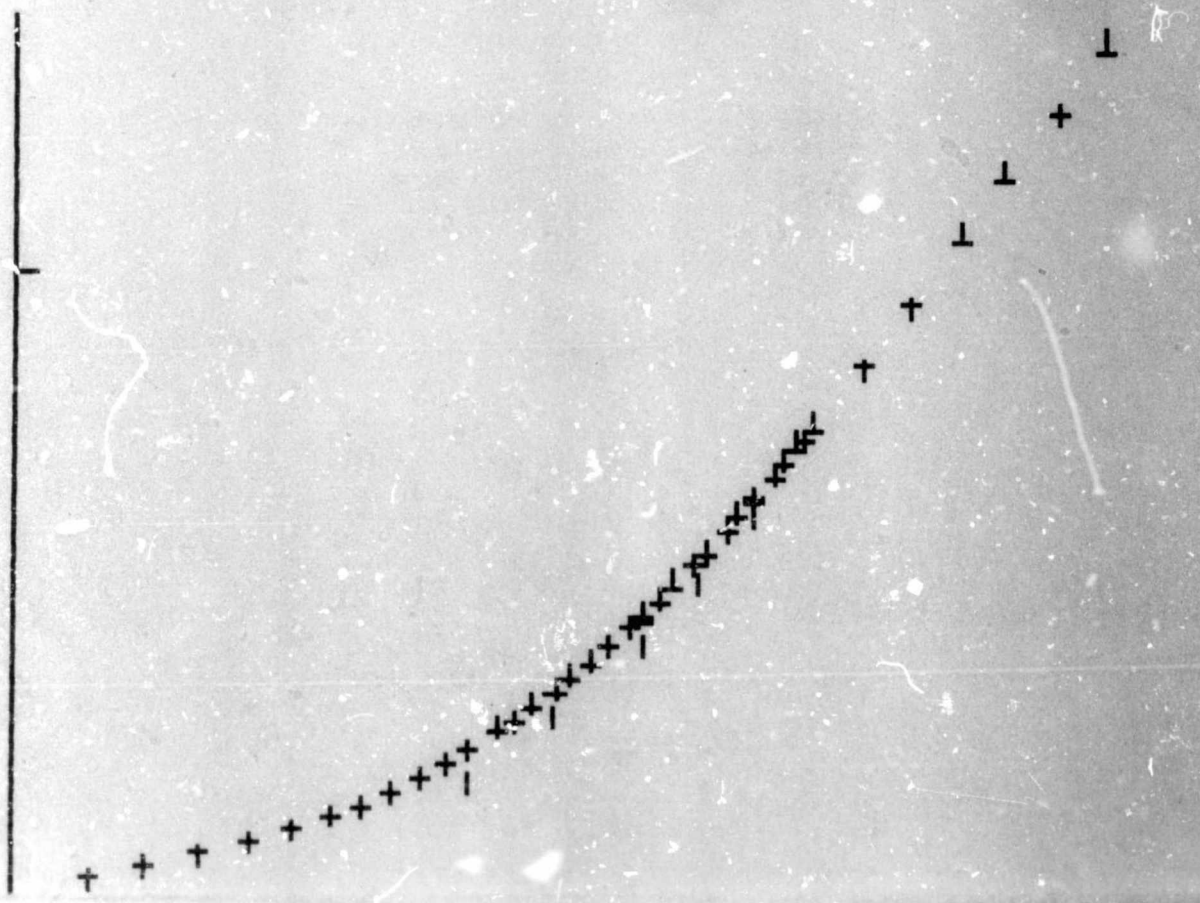
TITRATION 2

X - AXIS STARTS AT -5.1 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

| = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

1.80	10.6	-4.68	0.06	0.06	0.00
1.90	7.8	-4.60	0.07	0.07	0.00
2.00	5.2	-4.54	0.08	0.08	0.00
2.10	2.9	-4.48	0.09	0.09	0.00
2.20	0.6	-4.42	0.10	0.10	0.00
2.30	-1.6	-4.37	0.11	0.11	0.00
2.40	-3.5	-4.33	0.12	0.12	0.00
2.50	-5.4	-4.29	0.13	0.13	0.00
2.64	-8.0	-4.24	0.15	0.14	0.00
2.70	-9.4	-4.21	0.15	0.15	0.00
2.80	-11.1	-4.18	0.17	0.16	0.00
2.90	-13.2	-4.13	0.18	0.18	0.00
3.00	-14.9	-4.11	0.19	0.18	0.00
3.10	-16.8	-4.07	0.20	0.20	0.00
3.20	-18.8	-4.04	0.21	0.21	0.00
3.32	-21.2	-4.00	0.23	0.22	0.00
3.40	-22.8	-3.98	0.24	0.23	0.00
3.50	-24.8	-3.95	0.25	0.24	0.00
3.60	-26.8	-3.93	0.26	0.26	-0.01
3.70	-29.4	-3.89	0.27	0.27	0.00
3.80	-31.5	-3.87	0.29	0.28	0.00
3.90	-34.3	-3.83	0.30	0.30	0.00
4.00	-36.7	-3.81	0.31	0.31	0.00
4.10	-39.6	-3.79	0.33	0.32	0.00
4.22	-43.7	-3.75	0.34	0.34	0.00
4.30	-46.5	-3.73	0.35	0.35	0.00
4.40	-50.6	-3.71	0.37	0.36	-0.01
4.50	-55.6	-3.68	0.38	0.38	-0.01

Log K1(SrII)-DHP-15-aneN2O3



ACID CONSTANTS:

PKA (1) = 8.30
PKA (2) = 7.62

MATRIX CONDITION NUMBER = 1.0000
CONVERGENCE IN *2* CYCLES
RMSD = .0074
SUM DELTA SQUARED = .00

PARAMETERS AND ERRORS

LOG K (1) = 3.463 +- .003

TITRATION 1

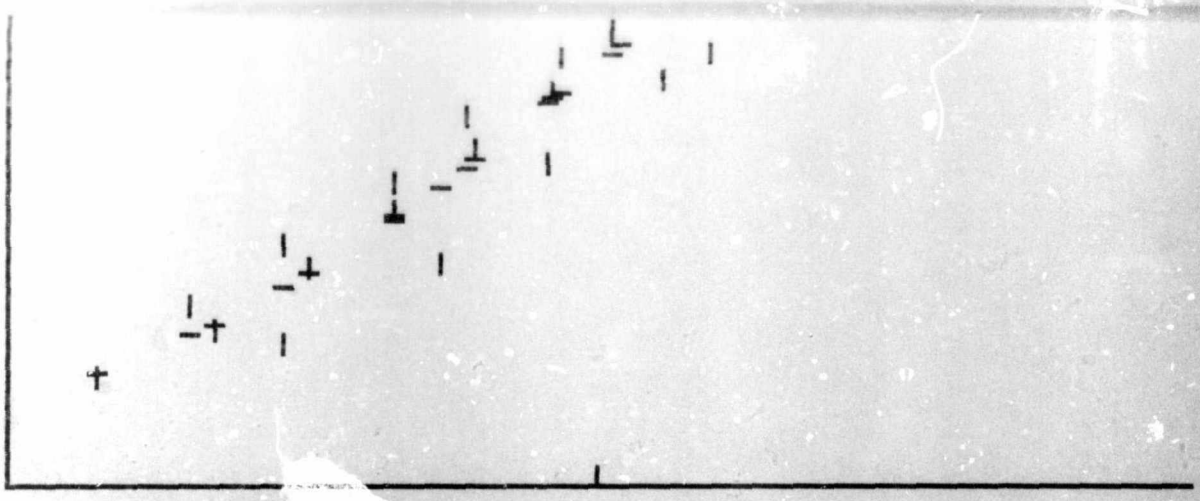
E0 /MV = 330.7
INIT VOL. /ML = 20.00
H+ IN CELL/MMOL = 0.25100
LIG IN CELL/MMOL = 0.09700
M IN CELL /MMOL = 0.06660
TITRANT B- /M = 0.05150

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.80	-87.2	-4.29	0.11	0.13	0.02
2.00	-93.0	-4.14	0.16	0.17	0.02
2.22	-99.2	-3.99	0.21	0.23	0.02
2.40	-103.6	-3.89	0.26	0.27	0.02
2.60	-108.3	-3.78	0.31	0.32	0.01
2.80	-112.7	-3.70	0.37	0.37	0.00
3.02	-118.4	-3.59	0.42	0.43	0.01
3.20	-122.9	-3.51	0.47	0.47	0.00
3.42	-128.3	-3.42	0.53	0.52	-0.01
3.60	-133.8	-3.34	0.58	0.57	-0.01
3.80	-140.6	-3.25	0.62	0.62	0.00
4.02	-148.4	-3.16	0.68	0.67	-0.01

TITRATION 2

E0 /MV = 417.1
INIT VOL /ML = 21.00
H+ IN CELL/MM... = 0.24900
LIG IN CELL/MMO... = 0.09700
M IN CELL /MMOL = ...19980
TITRANT B- /M = 0.050...

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.50	...0.8	-4.96	0.03	0.03	0.00
1.60	17.3	-4.86	0.04	0.04	0.00
1.70	13.7	-4.76	0.05	0.05	0.00



X - AXIS STARTS AT -0.9 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

! = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

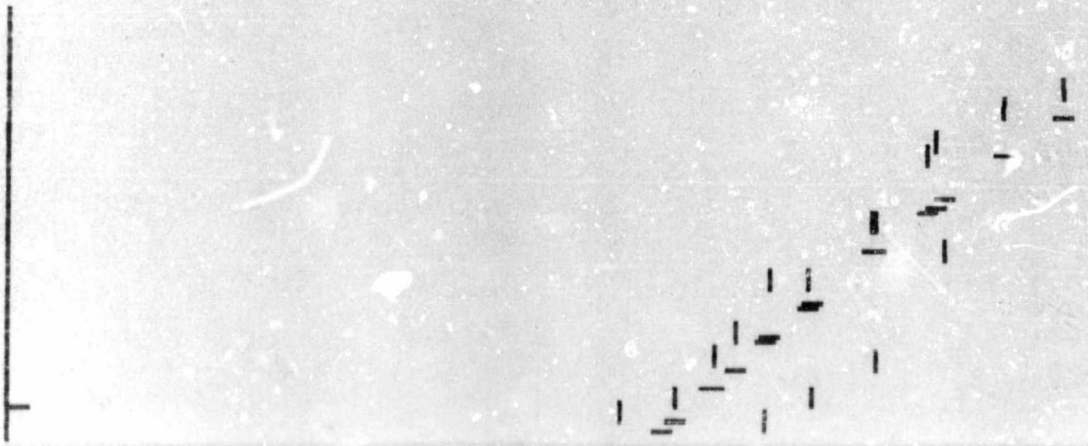
V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.62	-71.7	-4.76	0.10	0.11	0.01
1.80	-78.1	-4.58	0.15	0.16	0.01
2.00	-83.6	-4.44	0.21	0.21	0.00
2.20	-88.8	-4.31	0.27	0.26	-0.01
2.40	-93.9	-4.19	0.33	0.32	-0.01
2.60	-98.9	-4.07	0.39	0.38	-0.01
2.80	-103.3	-3.98	0.45	0.43	-0.02
3.00	-108.2	-3.88	0.51	0.49	-0.02
3.20	-113.0	-3.79	0.58	0.54	-0.04
3.40	-118.9	-3.63	0.63	0.60	-0.03
3.60	-125.0	-3.58	0.69	0.66	-0.03
3.80	-130.7	-3.50	0.75	0.70	-0.05
4.00	-138.8	-3.39	0.80	0.75	-0.05

TITRATION 3

E0	/MV	=	332.5
INIT VOL	/ML	=	19.00
LIG IN CELL	/MMOL	=	0.07298
M IN CELL	/MMOL	=	0.06660
TITRANT H+	/M	=	0.05019

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
0.20	-165.2	-3.29	0.82	0.79	-0.03
0.40	-143.2	-3.49	0.77	0.70	-0.06
0.60	-132.7	-3.58	0.69	0.66	-0.03
0.80	-122.4	-3.74	0.63	0.57	-0.06
1.00	-116.0	-3.83	0.56	0.52	-0.03
1.20	-108.6	-3.97	0.50	0.44	-0.05
1.40	-103.4	-4.06	0.43	0.39	-0.04
1.60	-96.9	-4.20	0.37	0.31	-0.05
1.80	-92.0	-4.31	0.30	0.26	-0.03
2.00	-85.3	-4.48	0.24	0.20	-0.04
2.20	-79.6	-4.62	0.18	0.15	-0.03

Log K1 $^{/CA/}_{****}$ -DHP-15-aneN2O3



Log K1(CaII)-DHP-15-aneN2O3

ACID CONSTANTS:

PKA (1) = 8.30
PKA (2) = 7.62

MATRIX CONDITION NUMBER = 1.0000
CONVERGENCE IN *3* CYCLES
RMSD = .0521
SUM DELTA SQUARED = .09

PARAMETERS AND ERRORS

LOG K (1) = 3.864 +- .018

TITRATION 1

E0	/MV	= 416.6
INIT VOL	/ML	= 20.00
H+ IN CELL	/MMOL	= 0.07530
LIG IN CELL	/MMOL	= 0.02910
M IN CELL	/MMOL	= 0.01650
TITRANT B-	/M	= 0.05150

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
0.60	-12.3	-4.48	0.14	0.20	0.06
0.70	-21.9	-4.24	0.22	0.30	0.08
0.80	-29.7	-4.07	0.32	0.38	0.06
0.90	-38.4	-3.90	0.40	0.48	0.08
0.94	-42.3	-3.83	0.43	0.52	0.09
1.00	-47.4	-3.75	0.49	0.57	0.08
1.04	-51.6	-3.68	0.51	0.60	0.09
1.10	-58.2	-3.58	0.55	0.66	0.11
1.20	-66.8	-3.48	0.66	0.71	0.05

TITRATION 2

E0	/MV	= 330.7
INIT VOL	/ML	= 20.00
H+ IN CELL	/MMOL	= 0.25109
LIG IN CELL	/MMOL	= 0.09714
M IN CELL	/MMOL	= 0.06650
TITRANT B-	/M	= 0.05150

E0	/MV	= 428.5
INIT VOL	/ML	= 18.00
H+ IN CELL	/MMOL	= 0.21795
LIG IN CELL	/MMOL	= 0.07265
M IN CELL	/MMOL	= 0.09990
TITRANT B-	/M	= 0.05010

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
2.00	148.2	-10.85	0.14	0.14	0.00
2.10	144.9	-10.76	0.17	0.17	0.00
2.20	142.0	-10.68	0.19	0.19	0.00
2.30	139.2	-10.61	0.21	0.22	0.00
2.40	136.6	-10.54	0.24	0.24	0.00
2.50	134.1	-10.48	0.26	0.27	0.01
2.60	131.8	-10.43	0.29	0.29	0.01
2.70	129.4	-10.38	0.31	0.32	0.01
2.80	127.3	-10.34	0.34	0.34	0.00
2.90	124.9	-10.29	0.36	0.37	0.00
3.00	122.6	-10.24	0.39	0.39	0.00
3.10	120.3	-10.20	0.41	0.42	0.00
3.20	118.2	-10.17	0.44	0.44	0.00
3.30	115.5	-10.12	0.46	0.46	0.00
3.40	113.5	-10.09	0.49	0.48	-0.01
3.50	110.2	-10.03	0.51	0.51	0.00
3.60	107.5	-10.00	0.54	0.53	-0.01
3.70	104.7	-9.97	0.56	0.55	-0.02
3.80	101.7	-9.94	0.59	0.56	-0.03
3.90	98.5	-9.92	0.61	0.57	-0.04

TITRATION 3

E0	/MV	= 443.4
INIT VOL	/ML	= 15.00
H+ IN CELL	/MMOL	= 0.21795
LIG IN CELL	/MMOL	= 0.07265
M IN CELL	/MMOL	= 0.16650
TITRANT B-	/M	= 0.05010

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
2.10	170.0	-11.03	0.10	0.10	0.00
2.20	167.4	-10.97	0.11	0.11	-0.01
2.30	164.9	-10.90	0.13	0.12	-0.01
2.40	162.9	-10.86	0.14	0.13	-0.01
2.50	160.3	-10.80	0.16	0.15	-0.01
2.60	158.3	-10.76	0.17	0.17	-0.01
2.70	156.1	-10.71	0.19	0.18	-0.01
2.80	154.1	-10.67	0.20	0.19	-0.01
2.90	152.2	-10.64	0.22	0.21	-0.01
3.00	150.3	-10.61	0.23	0.22	-0.02
3.10	148.4	-10.58	0.25	0.23	-0.02
3.20	146.3	-10.55	0.26	0.24	-0.02
3.30	144.3	-10.52	0.28	0.25	-0.02
3.40	142.2	-10.50	0.29	0.27	-0.03
3.50	139.9	-10.47	0.31	0.28	-0.03

Log K1(CdII)-15-ane-N3O2

ACID CONSTANTS:

PKA (1) = 9.29
PKA (2) = 8.50
PKA (3) = 2.12

MATRIX CONDITION NUMBER = 1.0006
CONVERGENCE IN *2* CYCLES
RMSD = .0139
SUM DELTA SQUARED = .01

PARAMETERS AND ERRORS

LOG K (1) = 10.053 +- .004

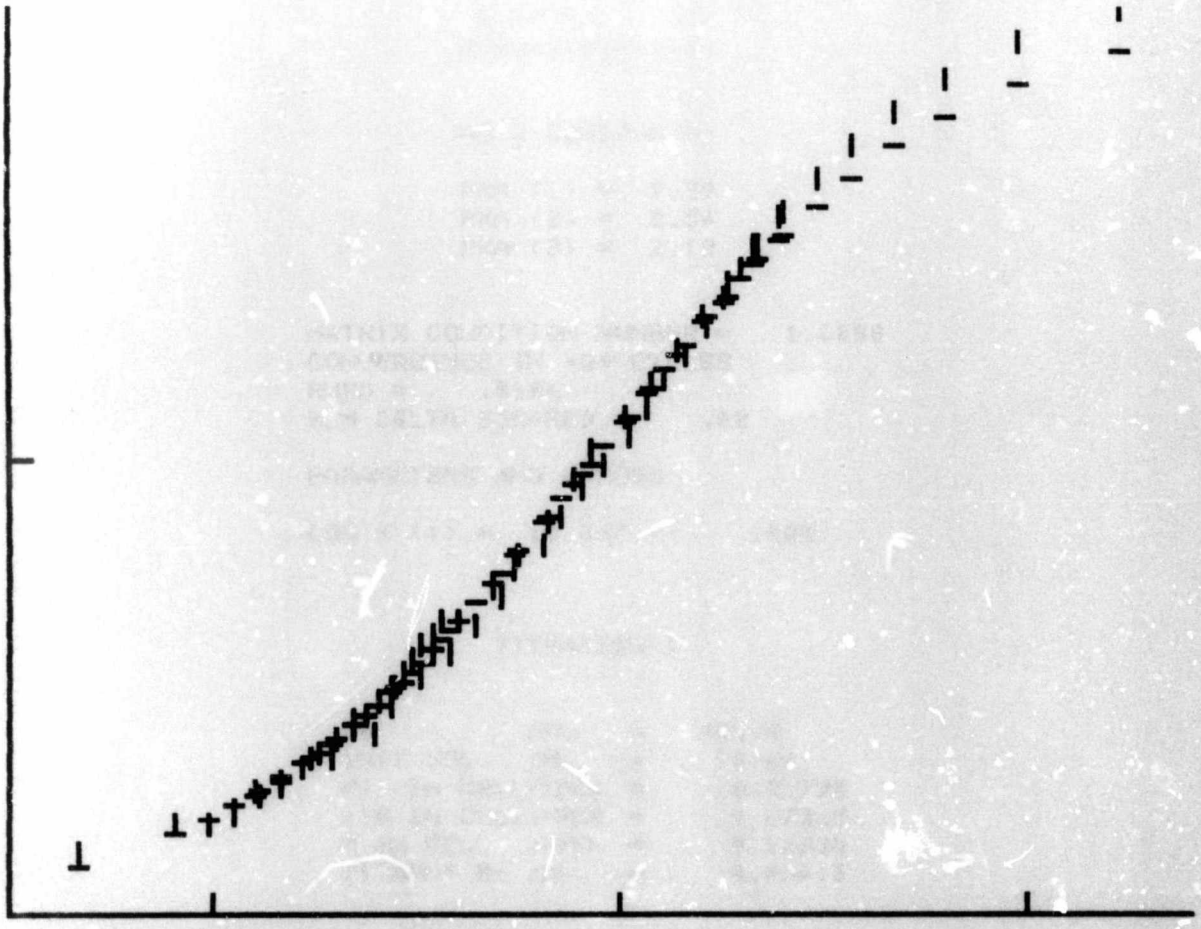
TITRATION 1

E0 /MV = 489.2
INIT VOL /ML = 17.00
H+ IN CELL/MMOL = 0.21795
LIG IN CELL/MMOL = 0.07265
M IN CELL /MMOL = 0.06660
TITRANT B- /M = 0.05010

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.70	134.7	-10.96	0.10	0.11	0.01
1.80	130.0	-10.82	0.14	0.15	0.01
1.90	125.6	-10.69	0.17	0.19	0.01
2.00	121.9	-10.59	0.21	0.23	0.02
2.10	118.8	-10.50	0.25	0.26	0.02
2.20	115.5	-10.41	0.28	0.30	0.02
2.30	112.9	-10.35	0.32	0.34	0.02
2.40	110.0	-10.27	0.36	0.38	0.02
2.50	107.4	-10.21	0.40	0.41	0.01
2.60	104.5	-10.14	0.43	0.45	0.02
2.70	101.8	-10.08	0.47	0.49	0.02
2.80	98.7	-10.00	0.51	0.53	0.02
2.90	96.3	-9.95	0.55	0.56	0.01
3.00	93.2	-9.88	0.58	0.60	0.02
3.10	90.3	-9.82	0.62	0.63	0.01
3.20	87.2	-9.75	0.66	0.67	0.01
3.30	83.7	-9.67	0.70	0.71	0.01
3.40	79.7	-9.58	0.73	0.75	0.01
3.50	76.5	-9.53	0.77	0.77	0.00
3.60	72.4	-9.44	0.81	0.80	-0.01
3.70	65.9	-9.29	0.85	0.85	0.01
3.80	61.0	-9.20	0.88	0.88	-0.01
3.90	52.9	-9.01	0.92	0.92	0.00
4.00	40.3	-8.70	0.96	0.96	0.00

TITRATION 2

Log K1(PbII)-15-ane-N3O2



X - AXIS STARTS AT -11.5 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

| = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.60	146.2	-11.33	0.06	0.05	-0.01
1.70	138.4	-11.09	0.10	0.09	-0.01
1.80	132.2	-10.90	0.14	0.13	-0.01
1.90	127.5	-10.76	0.17	0.17	0.00
2.00	123.8	-10.65	0.21	0.21	0.00
2.10	120.2	-10.55	0.25	0.25	0.00
2.20	116.7	-10.45	0.28	0.29	0.01
2.30	114.2	-10.39	0.32	0.32	0.00
2.40	111.0	-10.31	0.36	0.36	0.01
2.50	108.4	-10.24	0.40	0.40	0.00
2.60	105.5	-10.17	0.43	0.44	0.01
2.72	102.8	-10.11	0.48	0.47	-0.01
2.80	100.9	-10.07	0.51	0.50	-0.01
2.90	97.5	-9.99	0.55	0.54	0.00
3.00	94.6	-9.93	0.58	0.58	0.00
3.10	91.8	-9.87	0.62	0.61	-0.01
3.20	88.6	-9.80	0.66	0.65	-0.01
3.30	85.7	-9.74	0.70	0.68	-0.02
3.40	82.3	-9.67	0.73	0.71	-0.02
3.50	78.7	-9.60	0.77	0.75	-0.03
3.60	74.7	-9.52	0.81	0.78	-0.03
3.70	70.3	-9.44	0.85	0.81	-0.04
3.80	65.0	-9.33	0.88	0.84	-0.04
3.90	58.6	-9.20	0.92	0.88	-0.04
4.00	50.2	-9.03	0.96	0.92	-0.04
4.10	38.3	-8.78	1.00	0.95	-0.05

TITRATION 3

E0	/MV	=	409.4
INIT VOL	/ML	=	20.00
H+ IN CELL	/MMOL	=	0.21795
LIG IN CELL	/MMOL	=	0.07265
M IN CELL	/MMOL	=	0.08325
TITRANT B-	/M	=	0.05010

V/ML	E/MV	LG	NBAR	TH	TH-NBAR
1.80	131.9	-10.94	0.11	0.12	0.01
1.90	128.1	-10.83	0.14	0.15	0.01
2.00	123.7	-10.70	0.17	0.19	0.02
2.10	120.1	-10.60	0.20	0.23	0.03
2.20	118.2	-10.56	0.23	0.24	0.02
2.30	115.3	-10.48	0.26	0.28	0.02
2.40	112.4	-10.41	0.29	0.31	0.02
2.50	109.9	-10.35	0.32	0.34	0.03
2.60	107.3	-10.29	0.35	0.38	0.03
2.70	105.5	-10.25	0.38	0.39	0.02
2.80	102.5	-10.18	0.41	0.43	0.03
2.90	100.3	-10.14	0.44	0.46	0.02
3.00	98.0	-10.09	0.47	0.48	0.02
3.10	95.3	-10.04	0.50	0.52	0.02
3.20	92.5	-9.98	0.53	0.55	0.02
3.30	90.0	-9.94	0.56	0.57	0.02
3.40	87.4	-9.90	0.59	0.60	0.01
3.50	84.3	-9.84	0.62	0.63	0.01
3.60	81.1	-9.79	0.65	0.65	0.01
3.70	78.1	-9.75	0.68	0.67	0.00
3.80	74.5	-9.70	0.71	0.70	-0.01
3.90	70.6	-9.66	0.74	0.72	-0.02
4.00	66.6	-9.62	0.77	0.74	-0.03

Log K1(PbII)-15-ane-N3O2

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ACID CONSTANTS:

PKA (1) = 9.29
PKA (2) = 8.50
PKA (3) = 2.12

MATRIX CONDITION NUMBER = 1.0000
CONVERGENCE IN *3* CYCLES
RMSD = .0184
SUM DELTA SQUARED = .02

PARAMETERS AND ERRORS

LOG K (1) = 10.067 +- .005

TITRATION 1

E0 /MV = 443.4
INIT VOL /ML = 15.00
H+ IN CELL/MMOL = 0.21795
LIG IN CELL/MMOL = 0.07265
M IN CELL /MMOL = 0.16650
TITRANT B- /M = 0.05010

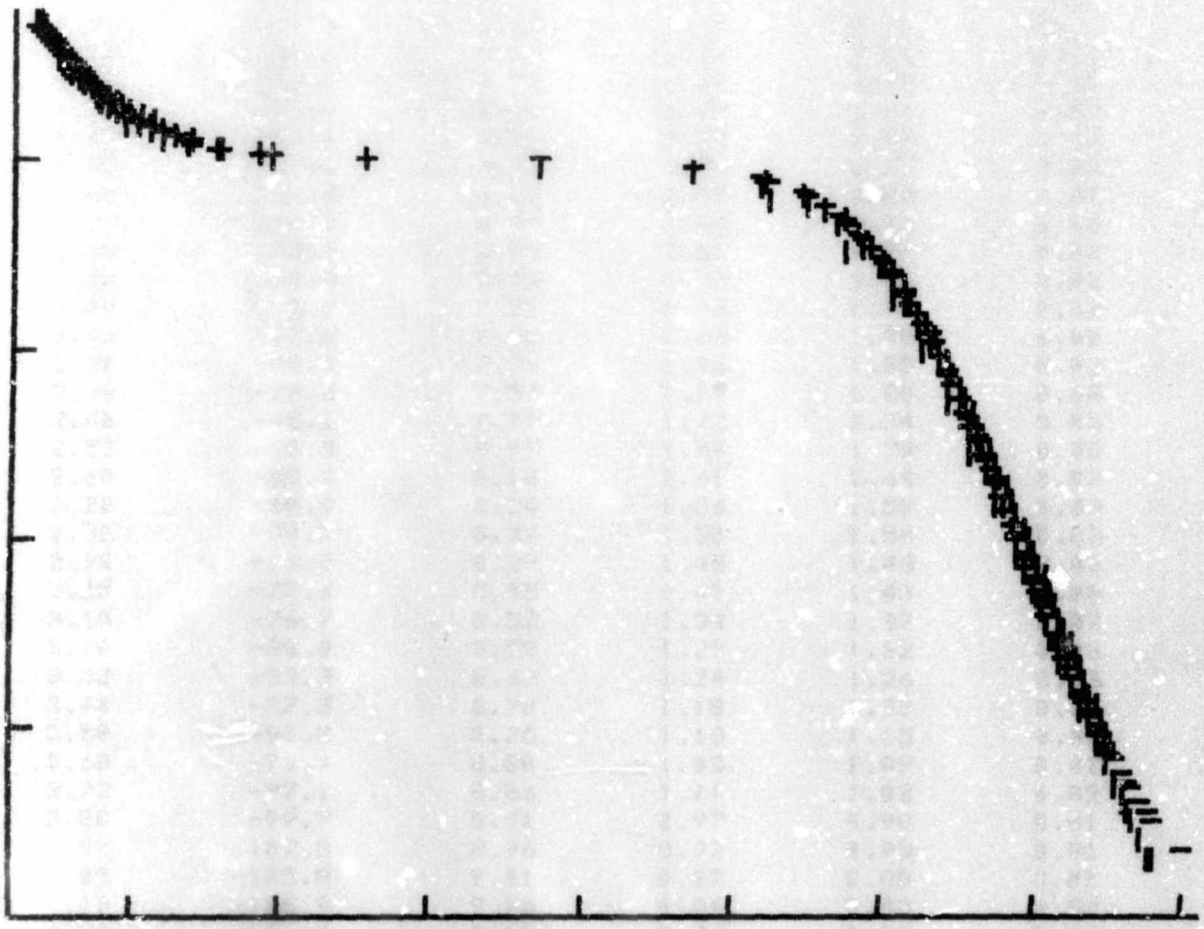
V/ML	E/MV	LG	NBAR	TH	TH-NBAR
2.10	169.4	-11.01	0.10	0.10	0.00
2.20	166.8	-10.94	0.11	0.12	0.00
2.30	164.3	-10.88	0.13	0.13	0.00
2.40	162.0	-10.83	0.14	0.15	0.00
2.50	159.7	-10.78	0.16	0.16	0.00
2.60	157.7	-10.74	0.17	0.18	0.00
2.70	155.6	-10.69	0.19	0.19	0.00
2.80	153.6	-10.65	0.20	0.21	0.00
2.90	151.7	-10.62	0.22	0.22	0.00
3.00	149.8	-10.59	0.23	0.23	0.00
3.10	147.9	-10.56	0.25	0.24	-0.01
3.20	145.9	-10.53	0.26	0.25	-0.01
3.30	143.9	-10.51	0.28	0.27	-0.01
3.40	141.8	-10.48	0.29	0.28	-0.02
3.50	139.6	-10.46	0.31	0.29	-0.02
3.60	137.2	-10.43	0.32	0.30	-0.02

TITRATION 2

E0 /MV = 409.2
INIT VOL /ML = 17.00
H+ IN CELL/MMOL = 0.21795
LIG IN CELL/MMOL = 0.07265
M IN CELL /MMOL = 0.16650
TITRANT B- /M = 0.05010

7.00	-144.6	9.35	0.61	0.56	-0.05
7.10	-146.7	9.39	0.58	0.53	-0.05
7.20	-148.7	9.42	0.54	0.50	-0.04
7.30	-150.7	9.46	0.51	0.47	-0.04
7.40	-152.8	9.49	0.48	0.45	-0.03
7.50	-154.4	9.52	0.44	0.43	-0.01

PKA-15-ane-N302



X - AXIS STARTS AT 2.2 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

! = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

V/ML	E/MV	PH	NBAR	TH	TH-NBAR
0.10	268.6	2.37	2.38	2.36	-0.02
0.20	267.6	2.39	2.36	2.35	-0.01
0.30	266.4	2.41	2.35	2.34	-0.01
0.40	265.2	2.43	2.34	2.33	-0.01
0.50	264.1	2.44	2.33	2.32	-0.01
0.60	262.6	2.47	2.32	2.31	-0.01
0.70	261.2	2.49	2.31	2.30	-0.01
0.80	259.8	2.52	2.29	2.28	-0.01
0.90	258.1	2.55	2.29	2.27	-0.01
1.00	256.8	2.57	2.27	2.26	-0.01
1.10	255.1	2.60	2.26	2.25	-0.01
1.20	253.4	2.63	2.25	2.24	-0.01
1.30	251.7	2.65	2.23	2.22	-0.01
1.40	249.7	2.69	2.22	2.21	-0.01
1.50	247.8	2.72	2.21	2.20	-0.01
1.60	245.7	2.76	2.19	2.19	-0.01
1.70	243.5	2.79	2.18	2.17	-0.01
1.80	240.8	2.84	2.17	2.16	-0.01
1.90	238.1	2.88	2.15	2.15	-0.01
2.00	235.3	2.93	2.14	2.13	-0.01
2.10	232.0	2.99	2.13	2.12	-0.01
2.20	228.2	3.05	2.11	2.10	-0.01
2.30	224.4	3.12	2.10	2.09	0.00
2.40	219.7	3.20	2.08	2.08	0.00
2.50	214.0	3.29	2.07	2.06	0.00
2.60	206.6	3.42	2.05	2.05	0.00
2.70	196.7	3.58	2.03	2.03	0.00
2.80	180.4	3.86	2.02	2.02	0.00
2.90	139.3	4.55	2.00	2.00	0.00
3.00	10.1	6.74	1.97	1.98	0.01
3.10	-19.1	7.23	1.94	1.95	0.01
3.20	-33.2	7.47	1.90	1.91	0.01
3.30	-42.6	7.63	1.87	1.88	0.01
3.40	-49.9	7.75	1.84	1.84	0.00
3.50	-55.8	7.85	1.80	1.80	0.00
3.60	-61.0	7.94	1.77	1.77	0.00
3.70	-65.1	8.01	1.73	1.73	0.00
3.80	-69.2	8.08	1.70	1.69	0.00
3.90	-73.2	8.15	1.66	1.65	-0.01
4.00	-76.4	8.20	1.63	1.62	-0.01
4.12	-79.2	8.25	1.59	1.59	0.00
4.20	-83.1	8.31	1.56	1.54	-0.02
4.30	-85.3	8.35	1.53	1.51	-0.02
4.40	-88.0	8.40	1.49	1.47	-0.02
4.50	-90.7	8.44	1.46	1.44	-0.02
4.60	-93.2	8.48	1.43	1.40	-0.03
4.70	-95.5	8.52	1.39	1.36	-0.03
4.80	-98.0	8.57	1.36	1.33	-0.03
4.90	-100.4	8.61	1.32	1.29	-0.04
5.00	-103.0	8.65	1.29	1.24	-0.04
5.10	-105.0	8.68	1.25	1.21	-0.04
5.20	-107.3	8.72	1.22	1.17	-0.05
5.30	-109.4	8.76	1.19	1.14	-0.05
5.40	-111.6	8.80	1.15	1.10	-0.05
5.50	-113.7	8.83	1.12	1.06	-0.06
5.60	-115.9	8.87	1.08	1.03	-0.06
5.70	-118.1	8.91	1.05	0.99	-0.06
5.80	-120.2	8.94	1.02	0.95	-0.07
5.90	-122.3	8.98	0.98	0.92	-0.07
6.00	-124.5	9.01	0.95	0.88	-0.07
6.10	-126.5	9.05	0.91	0.84	-0.07
6.20	-128.6	9.08	0.88	0.81	-0.07
6.30	-130.2	9.11	0.85	0.78	-0.07
6.40	-132.8	9.15	0.81	0.74	-0.07
6.50	-134.7	9.19	0.78	0.71	-0.07
6.60	-136.6	9.22	0.74	0.68	-0.07
6.70	-138.7	9.25	0.71	0.64	-0.07
6.80	-140.5	9.28	0.68	0.62	-0.06
6.90	-142.6	9.32	0.64	0.59	-0.06

V/ML	E/MV	PH	NBAR	TH	TH-NBAR
0.10	279.3	2.50	2.27	2.29	0.02
0.20	277.6	2.53	2.26	2.28	0.02
0.30	275.9	2.56	2.24	2.27	0.02
0.40	274.0	2.59	2.23	2.25	0.02
0.50	272.0	2.63	2.21	2.24	0.02
0.60	269.8	2.66	2.20	2.22	0.02
0.80	265.0	2.74	2.17	2.19	0.02
0.90	262.3	2.79	2.16	2.18	0.02
1.00	259.3	2.84	2.14	2.16	0.02
1.10	256.1	2.89	2.12	2.14	0.02
1.22	252.3	2.96	2.10	2.13	0.03
1.30	248.1	3.03	2.09	2.11	0.02
1.40	243.1	3.11	2.08	2.09	0.02
1.50	237.2	3.21	2.06	2.07	0.02
1.60	227.8	3.37	2.05	2.05	0.01
1.70	214.9	3.59	2.03	2.03	0.00
1.80	193.6	3.95	2.01	2.01	0.00
1.90	88.8	5.72	1.98	2.00	0.02
2.00	0.9	7.21	1.93	1.95	0.02
2.10	-17.0	7.51	1.88	1.90	0.03
2.20	-28.9	7.71	1.82	1.85	0.03
2.30	-38.2	7.87	1.77	1.80	0.03
2.40	-45.1	7.99	1.72	1.74	0.03
2.50	-50.3	8.07	1.66	1.70	0.03
2.60	-55.6	8.16	1.61	1.64	0.03
2.70	-60.4	8.24	1.56	1.59	0.03
2.80	-64.7	8.32	1.50	1.54	0.03
2.90	-68.8	8.39	1.45	1.48	0.03
3.00	-72.6	8.45	1.40	1.43	0.03
3.10	-76.7	8.52	1.34	1.37	0.02
3.20	-80.0	8.58	1.29	1.32	0.03
3.30	-83.3	8.63	1.24	1.26	0.03
3.40	-87.3	8.70	1.18	1.20	0.01
3.50	-90.3	8.75	1.13	1.15	0.02
3.60	-93.4	8.80	1.08	1.09	0.02
3.72	-97.1	8.86	1.01	1.03	0.02
3.80	-99.7	8.91	0.97	0.98	0.01
3.90	-102.8	8.96	0.92	0.93	0.01
4.00	-105.8	9.01	0.87	0.88	0.01
4.10	-108.8	9.06	0.81	0.83	0.02
4.20	-111.4	9.11	0.76	0.79	0.03
4.30	-115.6	9.18	0.71	0.72	0.01
4.40	-118.5	9.23	0.65	0.67	0.02
4.50	-121.4	9.27	0.60	0.63	0.02
4.62	-124.7	9.33	0.54	0.58	0.04
4.70	-127.7	9.38	0.50	0.53	0.04
4.80	-130.9	9.44	0.45	0.49	0.04
4.90	-134.0	9.49	0.39	0.45	0.06
5.02	-137.8	9.55	0.33	0.40	0.07
5.10	-141.0	9.61	0.29	0.37	0.08
5.20	-144.3	9.66	0.24	0.33	0.09
5.30	-147.8	9.72	0.19	0.30	0.11
5.40	-151.6	9.79	0.14	0.26	0.12

TITRATION 3

E0	/MV	=	408.7
INIT VOL	/ML	=	20.00
H+ IN CELL	/MMOL	=	0.43890
LIG IN CELL	/MMOL	=	0.14630
TITRANT B-	/M	=	0.05010

PKA-15-ane-N3O2

MATRIX CONDITION NUMBER = 3.0159
CONVERGENCE IN *3* CYCLES
RMSD = .0421
SUM DELTA SQUARED = .26

PARAMETERS AND ERRORS

PKA (1) = 9.291 +- .013
PKA (2) = 8.496 +- .013
PKA (3) = 2.116 +- .017

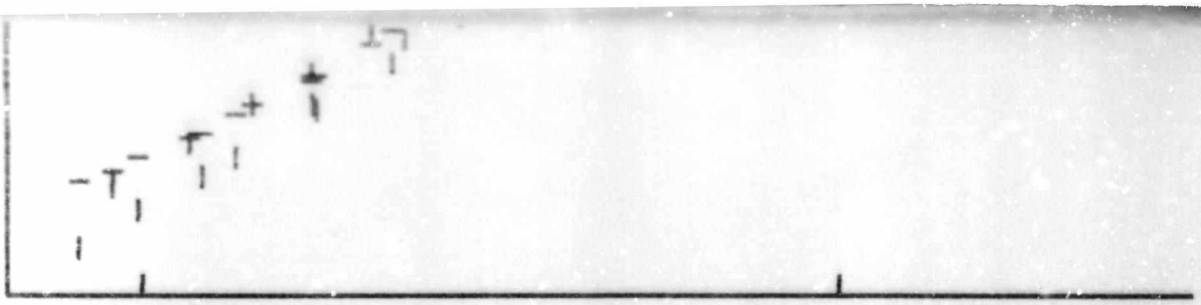
TITRATION 1

E0 /MV = 409.4
INIT VOL /ML = 20.00
H+ IN CELL/MMOL = 0.21795
LIG IN CELL/MMOL = 0.07265
TITRANT B- /M = 0.05010

V/ML	E/MV	PH	NBAR	TH	TH-NBAR
0.20	252.7	2.65	2.24	2.23	-0.01
0.40	248.3	2.72	2.19	2.20	0.01
0.60	242.0	2.83	2.17	2.16	0.00
0.80	235.2	2.94	2.12	2.13	0.01
1.00	228.9	3.04	2.10	2.09	-0.01
1.20	206.1	3.40	2.06	2.05	-0.01
1.40	176.5	3.94	2.00	2.01	0.01
1.60	-20.5	7.27	1.90	1.94	0.05
1.80	-50.6	7.78	1.76	1.83	0.07
2.00	-68.2	8.07	1.62	1.70	0.08
2.20	-80.1	8.27	1.48	1.57	0.08
2.40	-90.6	8.45	1.35	1.43	0.08
2.60	-99.3	8.60	1.21	1.29	0.08
2.80	-108.9	8.76	1.07	1.13	0.06
3.00	-116.6	8.89	0.94	1.00	0.07
3.20	-126.6	9.06	0.80	0.83	0.03
3.40	-134.5	9.19	0.66	0.70	0.04
3.60	-142.5	9.33	0.53	0.58	0.05
3.80	-152.8	9.50	0.40	0.44	0.04
4.00	-161.3	9.65	0.27	0.34	0.08
4.20	-171.2	9.81	0.14	0.25	0.11
4.40	-182.0	10.00	0.02	0.17	0.15

TITRATION 2

E0 /MV = 427.3
INIT VOL /ML = 20.00
H+ IN CELL/MMOL = 0.28107
LIG IN CELL/MMOL = 0.09369
TITRANT B- /M = 0.05010



X - AXIS STARTS AT -5.2 UNITS = 1.0
Y - AXIS STARTS AT 0 UNITS = 0.5

! = EXPERIMENTAL NBARS
_ = THEORETICAL NBARS

Author Bhavan Rekha
Name of thesis Ligand Design Using The Neutral Oxygen Donor To Control Metal Ion Size Selectivity. 1989

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