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ต้นฉบับ หน้าขาดหาย

Appendix A

Surface characterization of goethite by XRD

The three dimensional structure of nonamorphous materials, such as minerals, is defined by regular, repeating planes of atoms that form a crystal lattice. When a focused x-ray beam interacts with these planes of atoms, part of the beam is diffracted by each mineral differently, depending on what atoms make up the crystal lattice and how these atoms are arranged. This makes X-Ray Powder Diffraction (XRD) a suitable technique for identification of various minerals.

For this method, Bragg's law was obeyed, i.e., $n\lambda = 2d \sin\theta$. For each (hkl) plane in the crystal, there is a discrete value of θ at which diffraction occurs. This angle depends on the interplanar spacing, d_{hkl} , and the characteristic wavelength of x-rays. From the XRD analysis, the plot of intensity vs 2θ shows peaks at specific d values with different intensities, the dominant ones of which characterise the mineral samples.

For the goethite sample, the dominance(110) diffraction peak at 4.17 $\overset{0}{A}$ and (021) diffraction peaks at 2.69 and 2.45 $\overset{0}{A}$ were found and shown in figure A.1.
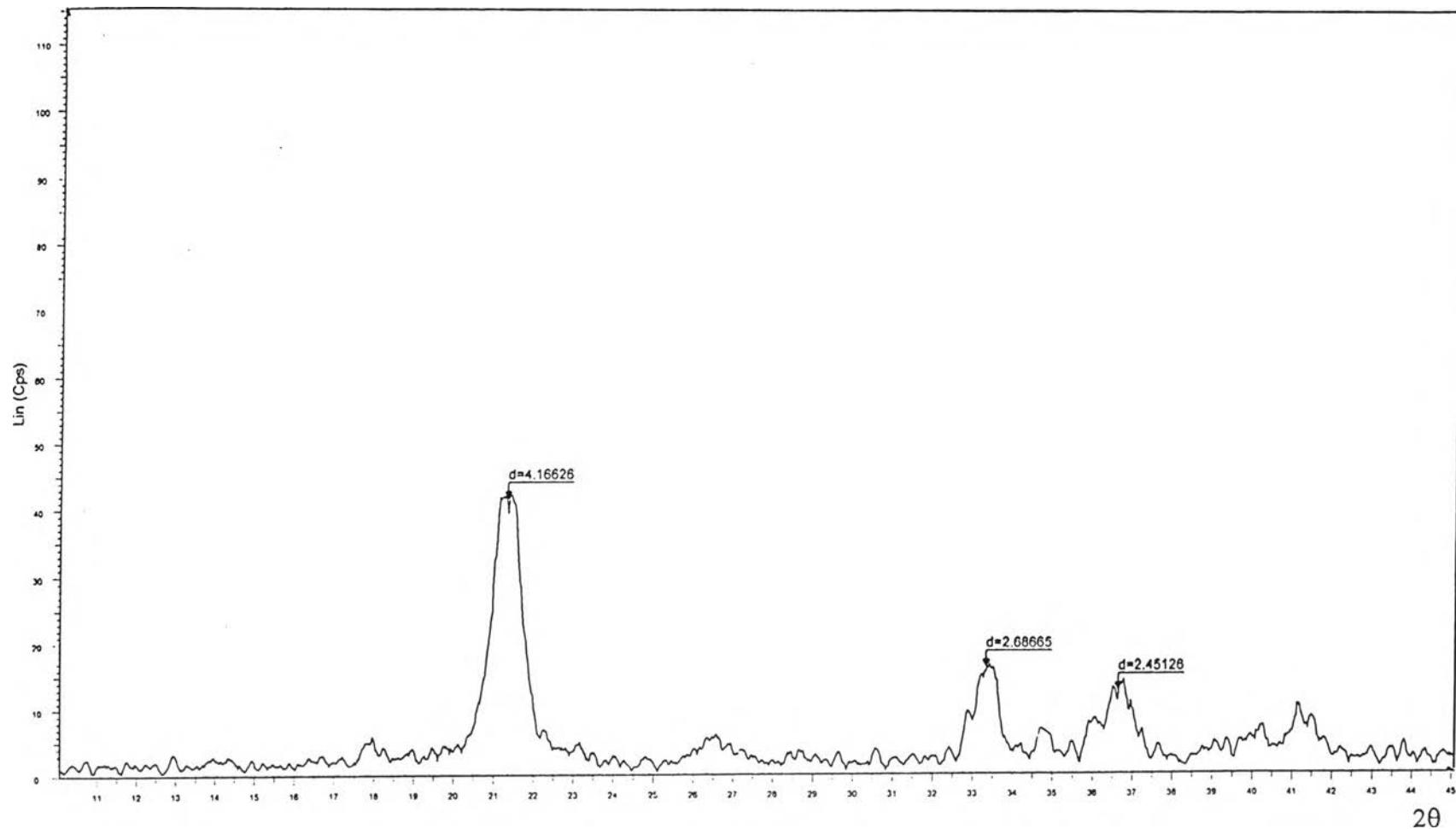
Figure A.1   XRD spectrum of goethite

Surface area determination of goethite

The most commonly used method to determine the specific surface area of powdered sample is the BET (Brunauer,Emmett, and Teller) N_2- adsorption method. With the exception of the assumption that the adsorption process terminates at monolayer coverage, the BET method retains all other assumptions made in deriving the Langmuir adsorption isotherm. This method allows for the adsorption in multilayers of gaseous atoms or molecules on top of the already adsorbed layer.

The linearized form of the BET equation can be written as,

$$\frac{P}{W(P_0-P)} = \frac{1}{W_m.C} + \frac{(C-1)}{W_m.C}.\frac{P}{P_0} \tag{1}$$

where P is the nitrogen gas pressure, P_0 is the saturation pressure, W is the volume of gas adsorbed, W_m is the volume of gas adsorbed in a monolayer and C is a constant related to the enthalpy of adsorption. This equation fits the adsorption data in the range $0 \leq P/P_0 \leq 0.30$. Rearranging equation (1) gives

$$\frac{1}{[W((P0/P)-1)]} = \frac{1}{W_m.C} + \frac{(C-1)}{W_m.C}.\frac{P}{P_0} \tag{2}$$

A plot of $1/[w((P_0/P)-1)]$ versus P/P_0 should thus yield a straight line with slope = $(C-1)/W_m$ .C and intercept = $1/W_m$.C. The specific surface area of powdered sample (S_A) is then calculated from the value of W_m:

$$S_A = N_A . \frac{W_m}{22,414} .S_0 / G \tag{3}$$

where N_A is the Avogadro constant, S_0 is the cross sectional area of nitrogen molecule (16.2 $Å^2$ /molecule) and G is the weight of the sample.

For the synthesized goethite sample obtained in this work, such a plot is shown in figure

A.2 and A.3, the average surface area is calculated to be 96.87 ± 0.2 m^2/g.
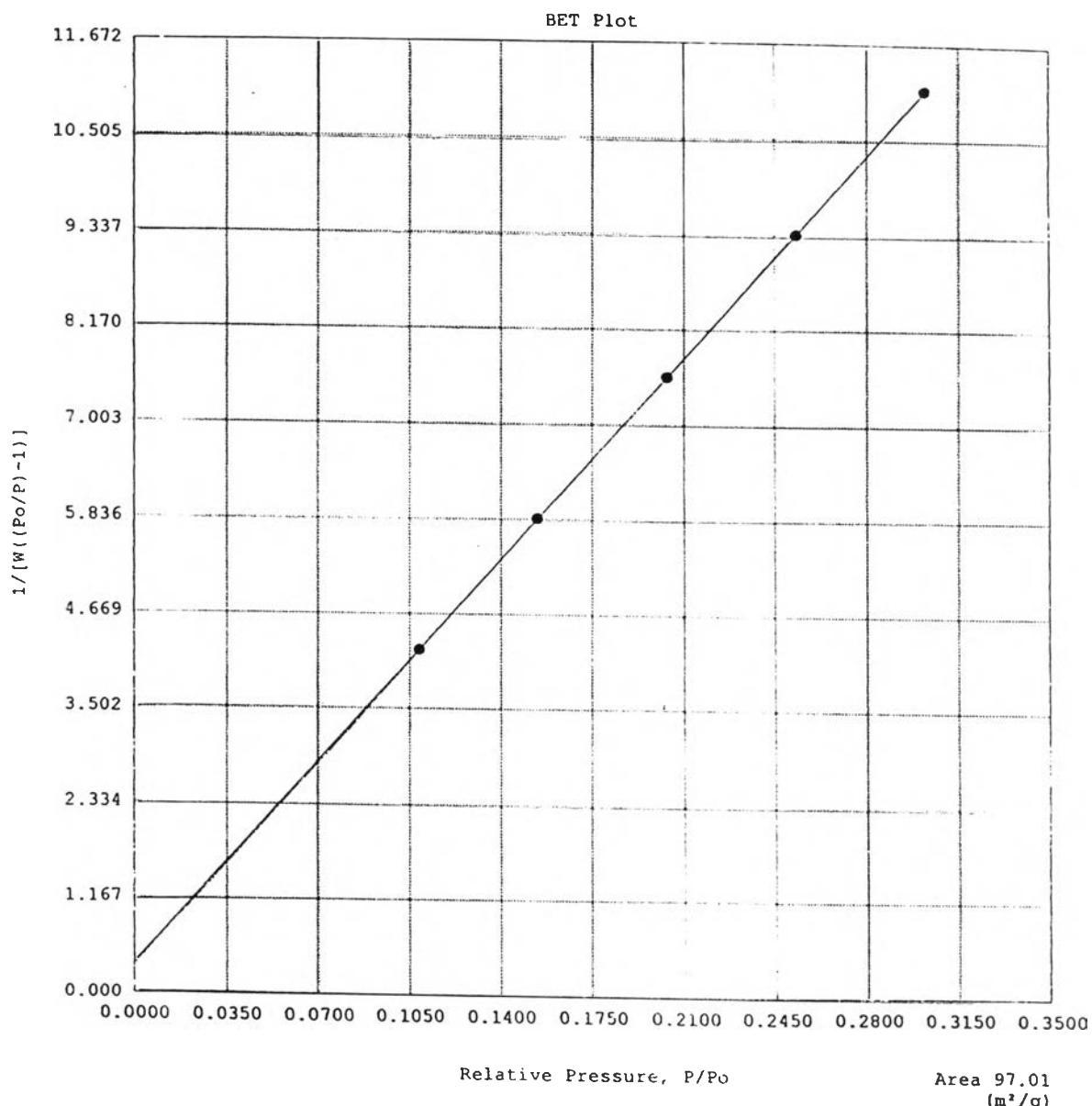
Figure A.2   BET plot for determination the surface area of goethite No.1.
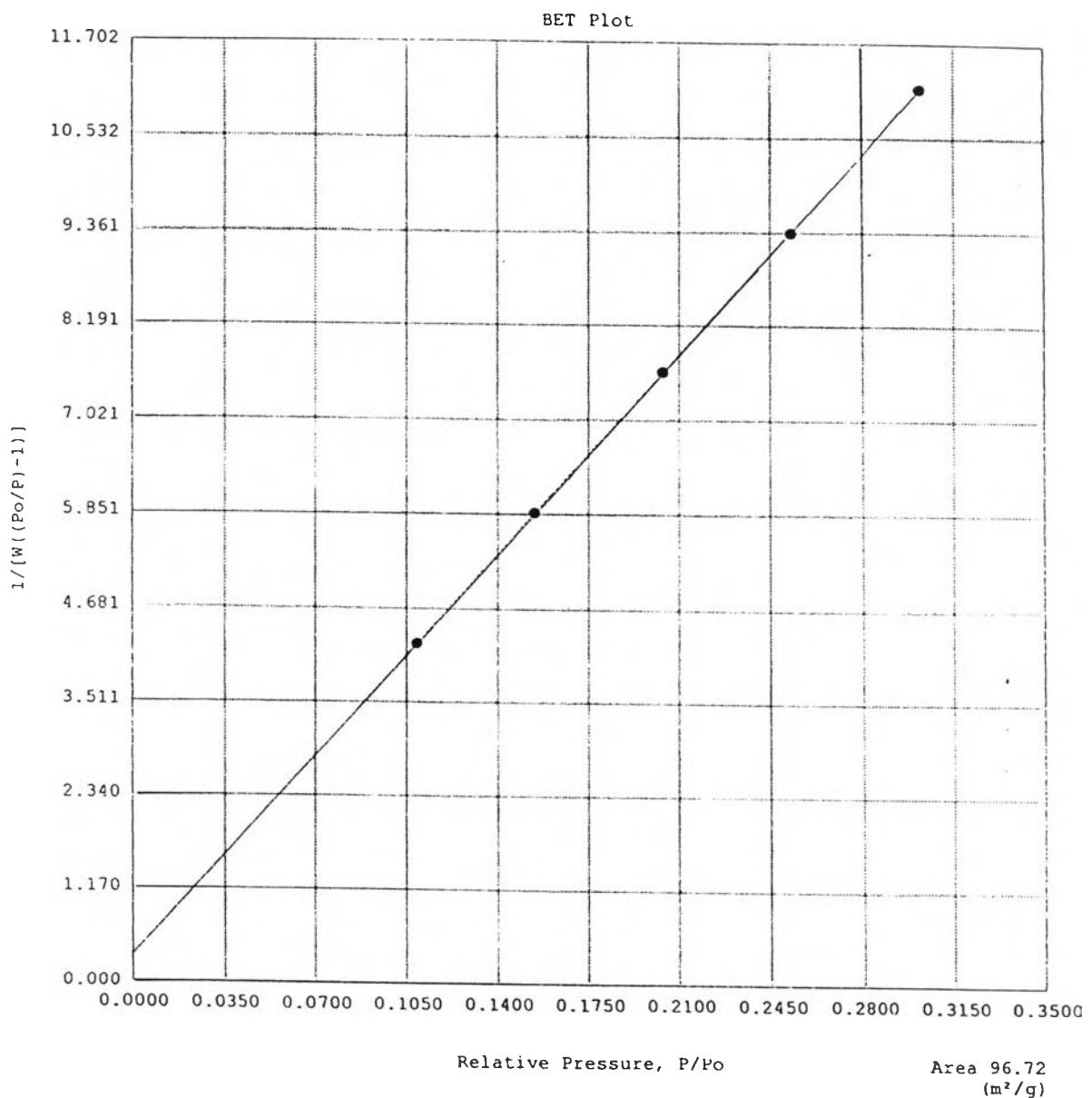
BET Plot

Figure A.3   BET plot for determination the surface area of goethite No.2.

APPENDIX B

The example of the titration curves for each system
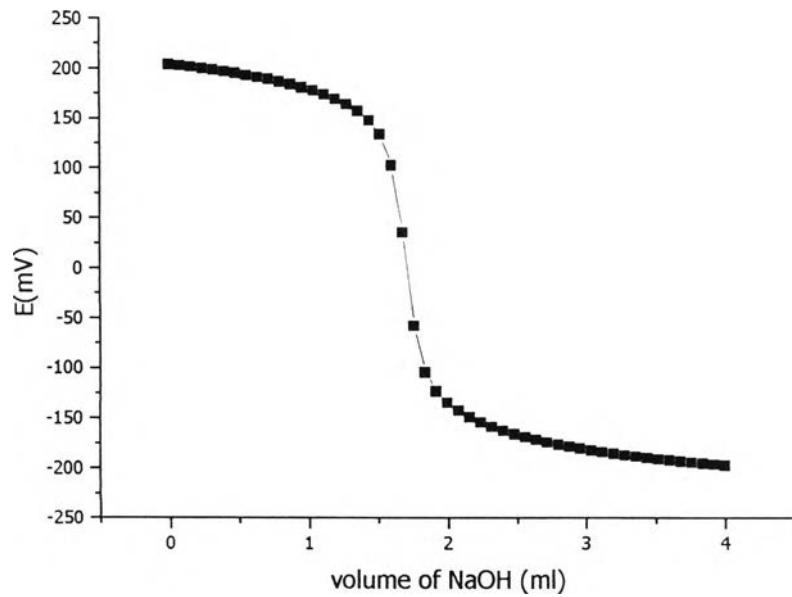
Figure B.1   Calibration curve for 0.100 M $NaNO_3$
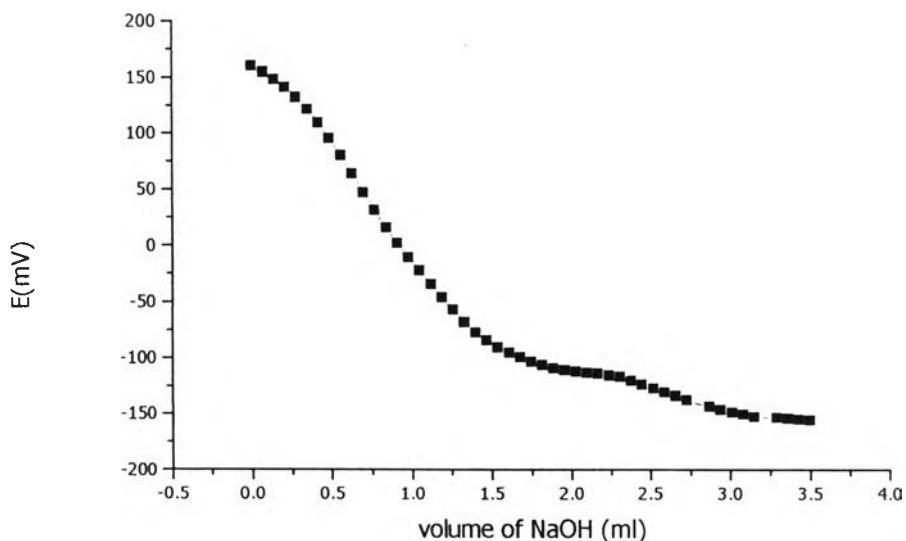
Figure B.2   Acid-base titration curve for 0.100 M $NaNO_3$
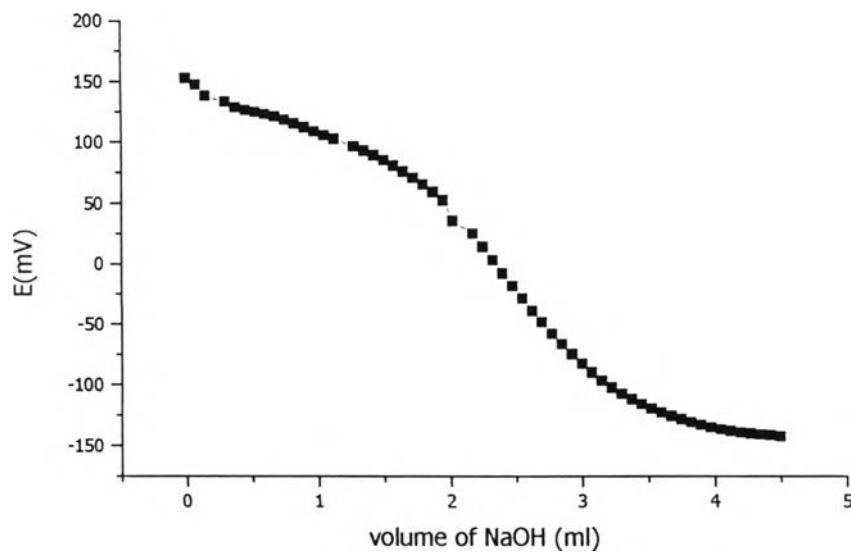
Figure B.3   Titration curve of goethite-H^+-Cu^{2+} system 0.100 M $NaNO_3$
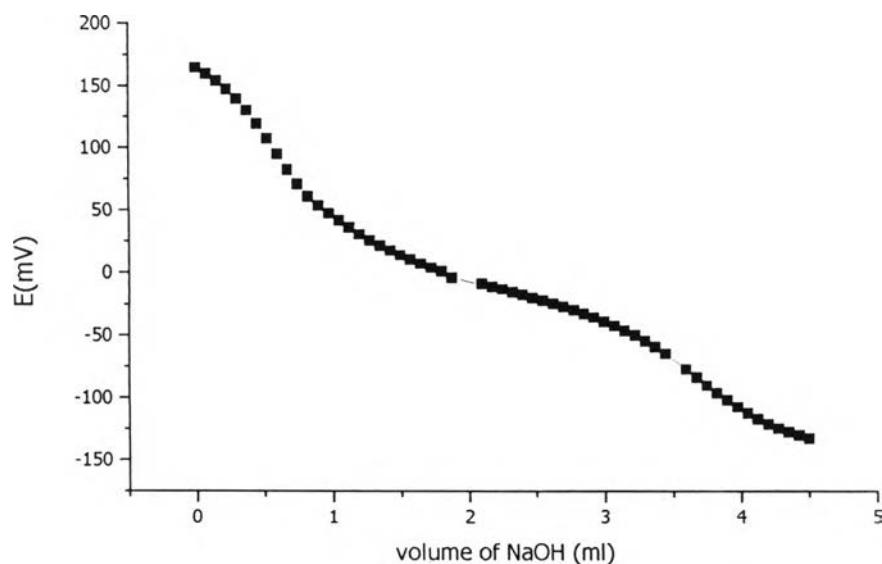
Figure B.4   Titration curve of goethite-H^+-Zn^{2+} system for 0.100 M $NaNO_3$
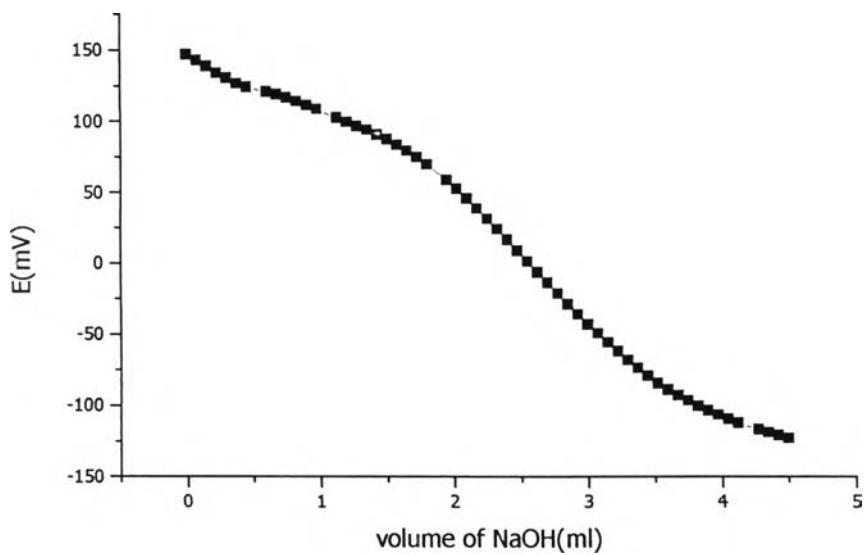
Figure B.5   Titration curve of goethite-H^+-Cu^{2+}-SO_4^{2-} system for 0.100 M $NaNO_3$
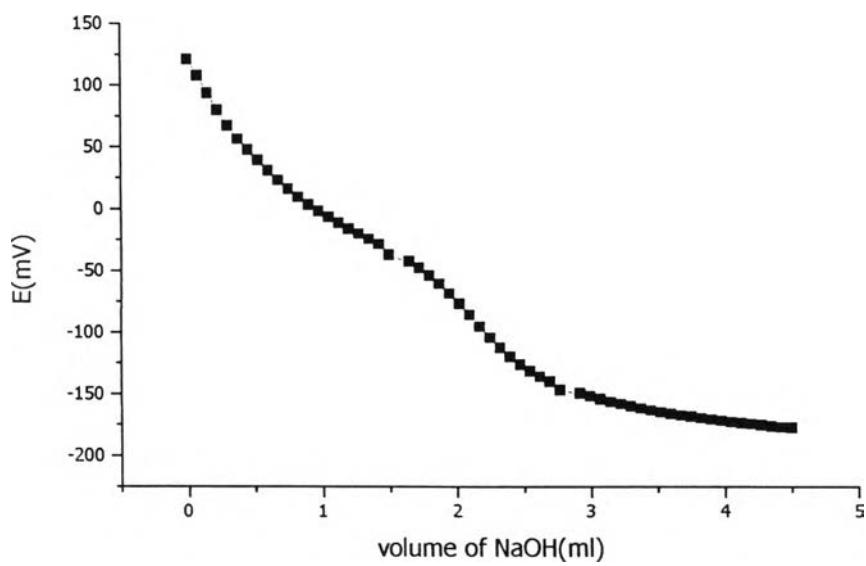
Figure B.6   Titration curve of goethite-H^+-Zn^{2+}-SO_4^{2-} system for 0.100 M $NaNO_3$

APPENDIX C

The example of input-output file for determination of the Standard Electrode Potential(E^0)

Calibration 0.500 M NaNO3 for Metal

99 2 1 3   [loop, print mode, no.of component, no]

proton

25.00 400.00 -400.00   .002   [temp.,starting mV, ended mV, no]

-13.77   -1   1   [log(K_w), H, RK(K_w)]

1 1   **.01000**   **-.01000** 1   1   [no,id., H^+ conc.(M),OH^- conc.(M), RK, RK]

0   **32.00000**   **2.00000**   [no, initial vol.in ves., H^+ vol.added in ves.]

0 1 1 **380.00000** .10000 **1**   .000   [no, RK, RK, initial guess E^0, ΔE, RK(E^0), RK]

0.0000 211.9	[titrant volume, reading mV]

0.0000 211.9   [titrant volume, reading mV]

0.0800 210.4

0.1600 208.9

0.2400 207.4

0.3200 205.9

0.4000 204.4

0.4800 202.8

0.5600 201.2

0.6400 199.4

0.7200 197.6

0.8000 195.7

0.8800 193.7

0.9600 191.5

1.0400	189.1	2.6400	-158.4
1.1200	186.5	2.7200	-161.6
1.2000	183.7	2.8000	-164.2
1.2800	180.4	2.8800	-166.5
1.3600	176.8	2.9600	-168.6
1.4400	172.6	3.0400	-170.5
1.5200	167.6	3.1200	-172.3
1.6000	161.5	3.2000	-174.0
1.6800	153.6	3.2800	-175.5
1.7600	142.2	3.3600	-177.0
1.8400	122.5	3.4400	-178.3
1.9200	69.2	3.5200	-179.6
2.0000	-17.4	3.6000	-180.8
2.0800	-99.6	3.6800	-182.0
2.1600	-121.2	3.7600	-183.1
2.2400	-132.4	3.8400	-184.0
2.3200	-140.4	3.9200	-184.9
2.4000	-146.2	4.0000	-185.9
2.4800	-151.1		
2.5600	-155.1		

ELECTRODE FITTING PROGRAME

V. 2.0, WINTER 1994

DEPT. OF INDUSTRIAL CHEMISTRY

WRITTEN BY DR. P. DOUNGDEE

KMIT LADKRABANG, BANGKOK 10520

PARAMETER TO BE FITED MORE THAN 3

IT POSIBLE YOU WILL GET WRONG RESULT

CONVERGENCE SATISFY AFTER 1 LOOPS

PARAMETERS CHANGE NOT MORE THAN .10 %

FINAL VALUES OF THE PARAMETERS :

CHI-SQR = 461.37625

PARAMETERS AND STANDARD DEV

PARAMETERS   380.20   .20000E-01 -.10000E-01 -12.842   46287. -.97816E-04

DEVIATION .67255E-06 .10499E-11 .52494E-12 .16238E-07 .26221E-02 .88401E-10

% DEVIATION .17689E-06 .52495E-08 -.52495E-08 -.12645E-06 .56649E-05 -.90375E-04

DEPENDENCIES -.18000E+14 -.18000E+14 -.18000E+14 -.18000E+14 -.18000E+14 -.18000E+14

CORRELATION COEFFICIENTS :

    A 1 1.0000

    A 2 .65586E-14 1.0000

    A 3 .65855E-14 -.50000E-13 1.0000

    A 4 -.35007E-13 -.28685E-15 -.35886E-15 1.0000

    A 5 -.30454E-13 -.18373E-15 -.76328E-16 .10662E-26 1.0000

    A 6 .21259E-13 .50062E-15 .54625E-15 .30364E-13 -.64756E-27   1.0000

DEGREES OF FREEDOM = 45

FINAL LAMBDA = .20000E+13

POINTS	EXP. MV	CAL. MV	RESIDUAL	PH
1	211.90	219.59	-7.6917	2.8451
2	210.40	217.25	-6.8524	2.8705
3	208.90	214.87	-5.9747	2.8958

4	207.40	212.45	-5.0545	2.9212
5	205.90	209.99	-4.0875	2.9465
6	204.40	207.47	-3.0682	2.9719
7	202.80	204.89	-2.0907	2.9989
8	201.20	202.25	-1.0479	3.0260
9	199.40	199.53	-.13177	3.0564
10	197.60	196.73	.86749	3.0868
11	195.70	193.84	1.8614	3.1190
12	193.70	190.84	2.8639	3.1528
13	191.50	187.71	3.7920	3.1900
14	189.10	184.43	4.6667	3.2305
15	186.50	180.99	5.5148	3.2745
16	183.70	177.33	6.3704	3.3218
17	180.40	173.42	6.9785	3.3776
18	176.80	169.20	7.6002	3.4385
19	172.60	164.58	8.0208	3.5095
20	167.60	159.43	8.1657	3.5940
21	161.50	153.57	7.9288	3.6971
22	153.60	146.66	6.9351	3.8306
23	142.20	138.11	4.0941	4.0234
24	122.50	126.53	-4.0264	4.3564
25	69.200	107.56	-38.362	5.2574
26	-17.400	-153.72	136.32	6.7213
27	-99.600	-101.31	1.7069	8.1109
28	-121.20	-121.20	.17033E-02	8.4760
29	-132.40	-132.27	-.12782	8.6653
30	-140.40	-139.96	-.44043	8.8006
31	-146.20	-145.85	-.35368	8.8986
32	-151.10	-150.61	-.48687	8.9815
33	-155.10	-154.62	-.48438	9.0491
34	-158.40	-158.06	-.33693	9.1049

35	-161.60	-161.09	-.51090	9.1589
36	-164.20	-163.78	-.41576	9.2029
37	-166.50	-166.21	-.28731	9.2418
38	-168.60	-168.42	-.17840	9.2773
39	-170.50	-170.45	-.53371E-01	9.3094
40	-172.30	-172.32	.15412E-01	9.3398
41	-174.00	-174.05	.49786E-01	9.3686
42	-175.50	-175.67	.16731	9.3939
43	-177.00	-177.18	.18233	9.4193
44	-178.30	-178.61	.30668	9.4413
45	-179.60	-179.95	.35028	9.4632
46	-180.80	-181.22	.42149	9.4835
47	-182.00	-182.43	.42746	9.5038
48	-183.10	-183.57	.47430	9.5224
49	-184.00	-184.67	.66734	9.5376
50	-184.90	-185.71	.81119	9.5528
51	-185.90	-186.71	.80991	9.5697

THE LAST RESULT OF CALCULATION

CONCENTRATION OF ACID =   .01000 SETRUN = 1

CONCENTRATION OF BASE =   -.01000 SETRUN = 1

FINAL   VALUE OF EZER =   380.20422 SETRUN = 1

FINAL   VALUE OF SLOP =   59.15572 SETRUN = 0

OR CORRECTED FACTER   =   1.00000

FINAL   VALUE OF WCON =   -12.84175 SETRUN = 1

FINAL   VALUE OF ACOR = 46287.   SETRUN = 1

FINAL   VALUE OF BCOR = -.97816E-04 SETRUN = 1

INITIAL VOLUME   =   32.00000

WORKING TEMPERATURE   =   25.00000

TOTAL NO. OF PARAMETERS WERE   FITED = 6

ต้นฉบับ หน้าขาดหาย

ต้นฉบับ หน้าขาดหาย

2. The system of goethite($\equiv$FeOH) - H$^+$- Cu^{2+}

GOETHITE-CU IN 0.500 M NANO3 <1:1:1>

99	3	3	2		[loop, print mode, no of comp., no]

CU — [metal]

GOETHTE — [ligand]

Hydrogen

25.00000 — [temperature]

8.80000	1	1	0	**1**	[log(β_1),no.metal,no.of ligand, H$^+$,RK]
0.90000	1	1	-1	**0**	[log(β_2),no.metal,no.of ligand, H$^+$,RK]
-6.60000	1	1	-2	**0**	[log(β_3),no.metal,no.of ligand, H$^+$,RK]
-8.12000	1	0	-1	**0**	[log($\beta_{hydrolysis}$),no.metal,no. of ligand,H$^+$,RK]
-8.95000	0	1	-1	**0**	[log(β_{a1}),no.metal,no. of ligand,H$^+$,RK]
6.31000	0	1	1	**0**	[log(β_{a2}),no.metal,no. of ligand,H$^-$,RK]
-12.91000	0	0	-1	**0**	[log(K_w),no.metal,no. of ligand,H$^+$,RK]

1 1	**0.01000**	0.00000	0	0	[no,id, mmol metal, mmol metal in bur.]
0 2	**0.01000**	0.00000	1	0	[no,id, mmol ligand, mmol ligand in bur.]
0 3	**0.01000**	-0.01000	1	1	[no,id, mmol acid, mmol base in bur.]

0	**32.00000**	0.01000		[no, initial vol.in ves., H$^+$ vol.added in ves.]
0 0 3	**405.61000**	0.05000	0 0	[no, RK, RK, initial guess E^0, ΔE, RK(E^0), RK]

0.000	138.9		0.450	113.0
0.075	134.9		0.525	109.5
0.150	130.3		0.600	107.3
0.225	125.5		0.675	105.5
0.300	121.0		0.750	103.3
0.375	117.1		0.825	100.9

0.900	98.2		2.775	-40.8
0.975	95.1		2.850	-46.7
1.050	91.6		2.925	-52.3
1.125	87.8		3.000	-57.3
1.200	84.0		3.075	-62.4
1.275	80.3		3.150	-67.3
1.350	76.5		3.225	-71.9
1.425	72.7		3.300	-77.2
1.500	68.6		3.375	-81.4
1.575	64.1		3.450	-85.8
1.650	59.0		3.525	-90.0
1.725	53.5		3.600	-93.6
1.800	47.6		3.675	-97.4
1.875	41.3		3.750	-101.1
1.950	34.5		3.825	-104.0
2.025	27.7		3.900	-107.3
2.100	20.6		3.975	-110.0
2.175	13.4		4.050	-112.7
2.250	6.3		4.125	-115.4
2.325	-0.6		4.200	-117.9
2.400	-7.6		4.275	-119.9
2.475	-14.6		4.35	-121.8
2.550	-21.6		4.425	-123.4
2.625	-28.1		4.500	-124.8
2.700	-34.6			

3. The system of Goethite($\equiv$FeOH) - H$^+$- Zn^{2+}

GOETHITE-Zn IN 0.500 M NANO3   <1:1:1> for metal

  99 3 3 2

Zn

GOETHTE

Hydrogen

  25.00000

  -2.00000 1 1 -1 1

  10.67000 1 2 0 1

-18.20000 1 1 -3 1

-17.10000 1 0 -1 0

  -8.95000 0 1 -1 0

  6.31000 0 1 1 0

-12.91000 0 0 -1 0

  1 1 0.01000 0.00000 1 0

  0 2 0.01000 0.00000 0 0

  0 3 0.01000 -0.01000 0 0

  0 32.00000 0.01000

0 0 3 405.61000 0.05000 0   0

0.000	141.3	0.600	68.2
0.075	133.2	0.675	60.5
0.150	124.2	0.750	53.8
0.225	114.4	0.825	48.1
0.300	104.6	0.900	43.1
0.375	94.7	0.975	38.1
0.450	85.3	1.050	33.1
0.525	76.3	1.125	28.3

1.200	23.8		3.525	-65.2
1.275	19.4		3.600	-67.8
1.350	15.1		3.675	-70.0
1.425	11.2		3.750	-72.1
1.500	7.5		3.825	-73.9
1.575	4.1		3.900	-75.9
1.650	0.7		3.975	-77.7
1.725	2.3		4.050	-79.9
1.800	-5.4		4.125	-82.3
1.875	-8.4		4.200	-84.9
1.950	-11.2		4.275	-87.2
2.025	-14.0		4.350	-89.1
2.100	-16.6		4.425	-90.7
2.175	-19.2		4.500	-91.9
2.250	-21.6			
2.325	-24.0			
2.400	-26.4			
2.475	-28.8			
2.550	-31.0			
2.625	-33.3			
2.700	-35.7			
2.775	-38.0			
2.850	-40.5			
2.925	-42.9			
3.000	-45.4			
3.075	-47.9			
3.150	-50.7			
3.225	-53.4			
3.300	-56.4			
3.375	-59.3			
3.450	-62.3			

4. The system of Goethite($\equiv$FeOH) - H$^+$- Cu^{2+}- SO$_4^{2-}$

GOETHITE-Cu-SO4 IN 0.500 M NANO3 <1:1:1> for metal

99 10 4 2

CU

GOETHTE

SULPHATE

Hydrogen

25.00000

13.00000	1	1	1	0	0
8.00000	1	1	1	-1	0
2.00000	1	1	1	-2	1
-8.12000	1	0	0	-1	0
4.87000	1	1	0	0	0
0.90000	1	1	0	-1	0
-6.60000	1	1	0	-2	0
8.30000	0	1	1	1	0
13.50000	0	1	1	2	0
-8.95000	0	1	0	-1	0
6.31000	0	1	0	1	0
-12.91000	0	0	0	-1	0

1 1	0.01000	0.00000	0	0
0 2	0.01000	0.00000	0	0
0 3	0.01000	0.00000	1	0
0 4	0.01000	-0.01000	0	1

0 33.00000 0.01000

0 0 3 405.61000 0.05000 0   0

0.000	150.6
0.075	145.5

0.150	140.3	2.400	-23.3
0.225	135.8	2.475	-30.8
0.300	131.4	2.550	-38.2
0.375	127.0	2.625	-44.8
0.450	124.3	2.700	-51.6
0.525	122.3	2.775	-58.1
0.600	120.1	2.850	-64.2
0.675	117.4	2.925	-69.7
0.750	114.4	3.000	-74.8
0.825	111.0	3.075	-79.5
0.900	107.5	3.150	-83.7
0.975	103.8	3.225	-87.1
1.050	100.2	3.300	-90.6
1.125	96.5	3.375	-94.0
1.200	93.1	3.450	-96.9
1.275	89.2	3.525	-99.9
1.350	84.8	3.600	-103.0
1.425	79.9	3.675	-105.9
1.500	74.6	3.750	-108.7
1.575	68.5	3.825	-110.8
1.650	61.8	3.900	-113.1
1.725	54.3	3.975	-115.2
1.800	46.1	4.050	-117.0
1.875	37.2	4.125	-118.9
1.950	27.7	4.200	-120.6
2.025	18.4	4.275	-122.4
2.100	9.1	4.350	-124.1
2.175	0.2	4.425	-125.7
2.250	-7.9	4.500	-127.2
2.325	-15.8		

5. The system of goethite($\equiv$FeOH) - H$^+$- Zn^{2+}- SO$_4$$^{2-}$

GOETHITE-Zn-SO4 IN 0.500 M NANO3 <1:1:1> for metal

 99   3   4   2

zn

GOETHTE

SULPHATE

Hydrogen

 25.00000

 11.64000   1   1   1 -1   1

 18.20000   1   2   1   0   0

 -2.50000   1   1   1 -3   0

-17.10000   1   0   0 -2   0

 -1.87000   1   1   0 -1   0

  8.71000   1   2   0   0   0

-16.35000   1   1   0 -3   0

  8.30000   0   1   1   1   0

 13.50000   0   1   1   2   0

 -8.95000   0   1   0 -1   0

  6.31000   0   1   0   1   0

-12.91000   0   0   0 -1   0

 1 1   0.01000   0.00000   1   0

 0 2   0.01000   0.00000   1   0

 0 3   0.01000   0.00000   1   0

 0 4   0.01000 -0.01000   1   1

  0 33.00000   0.01000

0 0 3 405.61000   0.05000   0   0

   0.000   128.7

   0.075   120.3

0.150	110.2	2.475	-35.4
0.225	100.7	2.550	-38.0
0.300	91.1	2.625	-40.6
0.375	81.7	2.700	-43.3
0.450	72.9	2.775	-46.1
0.525	64.7	2.850	-48.9
0.600	57.4	2.925	-51.9
0.675	51.2	3.000	-54.9
0.750	45.6	3.075	-58.1
0.825	40.1	3.150	-61.5
0.900	34.6	3.225	-64.8
0.975	29.3	3.300	-68.6
1.050	24.3	3.375	-72.4
1.125	19.6	3.450	-76.5
1.200	15.3	3.525	-80.2
1.275	11.2	3.600	-84.0
1.350	7.2	3.675	-87.7
1.425	3.5	3.750	-91.4
1.500	0.0	3.825	-94.9
1.575	-3.2	3.900	-98.3
1.650	-6.6	3.975	-101.6
1.725	-9.6	4.050	-104.7
1.800	-12.5	4.125	-107.7
1.875	-15.2	4.200	-110.4
1.950	-17.8	4.275	-112.9
2.025	-20.4	4.350	-115.2
2.100	-23.0	4.425	-117.2
2.175	-25.5	4.500	-119.3
2.250	-27.9		
2.325	-30.5		
2.400	-33.0		

APPENDIX E

The example of the output for Superquad program

1.The acid-base system

SUPERQUAD PROGRAM
V 2.0 Winter 1994 adopt from V 1984A
by Dr. P. Doungdee KMITL
Deprotonation and protonation of GOETHITE

MAXIT IPRIN MODE TOL ACCM RELAC
99 5 3 .10E-03 .10E-74 .298023E-07
REACTANT 1- GOETHITE 0.
REACTANT 2- proton
THE TEMPERATURE OF SOLUTION(S) IS 25.00 DEGREES CENTIGRADE
THE TITRATIONS ARE IN RANGE 400.0 TO -400.0 (IN MV)
THE SD-LIMITS =   .99

	FORMATION CONSTANTS	LOG BETAS'	REFINEMENT KEYS	STOICHIOMETRIC COEFFICIENTS
A	.3090E -9	-9.5100	1	1 -1
B	2.9512E 7	7.4700	1	1 1
C	.1698E-13	-13.7700	0	0 -1

2 FORMATION CONSTANTS TO BE REFINED
SLOPE =   59.15791
CURVE 1 INITIAL VOLUME 31.00
 1 SPECIAL PARAMETERS TO BE REFINED
                 CURVE   VALUE
   EZERO proton   1   3.8000E+02
100 ITERATIONS IN CCFR AT POINT 1
ITERATION 1 SIGMA= 15.10895   SUM OF SQUARES = 1.0957E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	.3090E -9	-.1869	2.5127E-10	1.9954
BETA B	2.9512E 7	-.9000	2.9512E 6	1.1568
CURVE 1 EZERO proton	3.8000E+02	.8020	4.1048E+02	.5559

ITERATION 3 SIGMA= .07914   SUM OF SQUARES = 3.0061E-01

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	1.6503E-10	.0038	1.6566E-10	.1318
BETA B	6.4256E 6	-.0006	6.4216E 6	.1155
CURVE 1 EZERO proton	4.4163E+02	-.0001	4.4163E+02	.0146

Deprotonation and protonation of GOETHITE
 3 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY

CHI-SQUARED = 4.06
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
 SIGMA =   .0791

	VALUE	REL STD DEV	LOG BETA		STD DEVIATION	
BETA A REFINED	1.65662E-10	.1318	**-9.9078**	.06139	1	-1
BETA B REFINED	6.42162E 6	.1155	**6.80764**	.05330	1	1
BETA C CONSTANT	.16982E-13		-13.77000		0	-1

		CURVE	INITIAL VALUE	FINAL VALUE	STD DEV
EZERO	**proton**	1	438.95396	**441.62888**	.64294

2. The system of goethite(≡FeOH) - H⁺- Cu²⁺

MAXIT IPRIN MODE TOL ACCM RELAC
99   10   2   .10E-03   .10E-74   .601347-153

REACTANT 1- Cu
REACTANT 2- GOETHTE
REACTANT 3- Hydrogen
THE TEMPERATURE OF SOLUTION(S) IS 25.00 DEGREES CENTIGRADE

	FORMATION CONSTANTS	LOG BETAS	REFINEMENT KEYS	STOICHIOMETRIC COEFFICIENTS		
A	6.3096E 8	8.8000	1	1	1	0
B	7.9433E 0	.9000	0	1	1	-1
C	.2512E -6	-6.6000	1	1	1	-2
D	.7586E -8	-8.1200	0	1	0	-1
E	.1660E -9	-9.7800	0	0	1	-1
F	6.4565E 6	6.8100	0	0	1	1
G	.1698E-13	-13.7700	0	0	0	-1

2 FORMATION CONSTANTS TO BE REFINED
CURVE 1 INITIAL VOLUME   32.00
        TITRE VOLUME ERROR   .01000 MILLILITRES

REACTANT	INITIAL NO OF MILLIMOLES	TITRANT MOLES/LITRE	STANDARD POTENTIAL MILLIVOLTS	ELECTRODE ERROR
Cu	.01000	.00000	NO ELECTRODE	
GOETHTE	.01000	.00000	NO ELECTRODE	
Hydrogen	.01000	-.01000	441.60000	.05000

2 SPECIAL PARAMETERS TO BE REFINED

		CURVE	VALUE
TOT MMOLES	Cu	1	1.0000E-02
TOT MMOLES	GOETHTE	1	1.0000E-02

100 ITERATIONS IN CCFR AT POINT 1
ITERATION 1 SIGMA= 152.24517   SUM OF SQUARES = 1.3212E+06

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.3096E 8	-.9000	6.3096E 7	2.4282
BETA C	.2512E -6	-.8268	4.3508E -8	3.9987

ITERATION 2 SIGMA= 130.76347   SUM OF SQUARES = 9.7465E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.3096E 7	-.9000	6.3096E 6	.9074
BETA C	4.3508E -8	-.7729	9.8810E -9	2.5158

100 ITERATIONS IN CCFR AT POINT 1

ITERATION   3 SIGMA= 94.69572   SUM OF SQUARES = 5.1113E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.3096E 6	-.9000	6.3096E 5	.6849
BETA C	9.8810E -9	-.4660	5.2763E -9	1.9167

ITERATION   4 SIGMA= 59.75277   SUM OF SQUARES = 2.0351E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.3096E 5	2.3390	2.1068E 6	1.2269
BETA C	5.2763E -9	-.5782	2.2256E -9	1.1286

ITERATION   5 SIGMA= 27.14661   SUM OF SQUARES = 4.2005E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.1068E 6	.1703	2.4655E 6	.4325
BETA C	2.2256E -9	-.5299	1.0462E -9	.4863

ITERATION   6 SIGMA= 16.46121   SUM OF SQUARES = 1.5445E+04
MARQUART PARAMETER FOR NEXT ITERATION 1.4180E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.4655E 6	.0526	2.5952E 6	.3218
BETA C	1.0462E -9	-.2567	7.7764E-10	.2893

ITERATION   7 SIGMA= 11.15983   SUM OF SQUARES = 7.0989E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.5952E 6	-.1609	2.1775E 6	.2384
BETA C	7.7764E-10	-.2792	5.6053E-10	.1981

ITERATION   8 SIGMA= 10.44303   SUM OF SQUARES = 6.2162E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.1775E 6	.1431	2.4890E 6	.2522
BETA C	5.6053E-10	.0369	5.8120E-10	.2221

ITERATION   9 SIGMA= 10.32681   SUM OF SQUARES = 6.0787E+03
MARQUART PARAMETER FOR NEXT ITERATION 2.3438E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.4890E 6	-.1100	2.2153E 6	.2393
BETA C	5.8120E-10	-.0626	5.4484E-10	.2008
CURVE 1 TOT MMOLES Cu	1.7076E-02	.0019	1.7080E-02	.1518
CURVE 1 TOT MMOLES GOETHTE	2.8059E-02	.1615	2.8513E-02	.3854

ITERATION 10 SIGMA= 10.29332   SUM OF SQUARES = 6.0393E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.2153E 6	.0538	2.3345E 6	.2503
BETA C	5.4484E-10	.0070	5.4866E-10	.2199

ITERATION 11 SIGMA= 10.28372   SUM OF SQUARES = 6.0280E+03
MARQUART PARAMETER FOR NEXT ITERATION 2.3438E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.3345E 6	-.0231	2.2805E 6	.2470
BETA C	5.4866E-10	-.0123	5.4193E-10	.2130

ITERATION 12 SIGMA= 10.28219   SUM OF SQUARES = 6.0262E+03
MARQUART PARAMETER FOR NEXT ITERATION 2.3438E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.2805E 6	.0104	2.3042E 6	.2490
BETA C	5.4193E-10	.0019	5.4296E-10	.2169

CHI-SQUARED = 1.03
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
   SIGMA =   9.1484

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION			
BETA A REFINED	2.04337E 6	.2227	**6.31035**	.10943	1	1	0
BETA B CONSTANT	7.94328E 0		**.90000**		1	1	-1
BETA C REFINED	4.86865E-10	.2353	**-9.31259**	.11650	1	1	-2
BETA D CONSTANT	.75858E -8		-8.12000		1	0	-1
BETA E CONSTANT	.16596E -9		-9.78000		0	1	-1
BETA F CONSTANT	6.45654E 6		6.81000		0	1	1
BETA G CONSTANT	.16982E-13		-13.77000		0	0	-1

3. The system of Goethite($\equiv$FeOH) - H^+- Zn^{2+}

MAXIT	IPRIN	MODE	TOL	ACCM	RELAC	
99	10	2	.10E-03	.10E-74	.601347-153	

REACTANT 1- Zn
REACTANT 2- GOETHTE
REACTANT 3- Hydrogen
THE TEMPERATURE OF SOLUTION(S) IS 25.00 DEGREES CENTIGRADE

	FORMATION CONSTANTS	LOG BETAS	REFINEMENT KEYS	STOICHIOMETRIC COEFFICIENTS		
A	1.0000E -2	-2.0000	1	1	1	-1
B	4.6774E 10	10.6700	1	1	2	0
C	.6310E-18	-18.2000	1	1	1	-3
D	.7943E-17	-17.1000	0	1	0	-2
E	.1660E -9	-9.7800	0	0	1	-1
F	6.4565E 6	6.8100	0	0	1	1
G	.1698E-13	-13.7700	1	0	0	-1

4 FORMATION CONSTANTS TO BE REFINED
CURVE 1 INITIAL VOLUME   32.00
TITRE VOLUME ERROR   .01000 MILLILITRES

REACTANT	INITIAL NO OF MILLIMOLES	TITRANT MOLES/LITRE	STANDARD POTENTIAL MILLIVOLTS	ELECTRODE ERROR
Zn	.01000	.00000	NO ELECTRODE	
GOETHTE	.01000	.00000	NO ELECTRODE	
Hydrogen	.01000	-.01000	441.60000	.05000

1 SPECIAL PARAMETERS TO BE REFINED

		CURVE	VALUE
ADDED CONC	Hydrogen	1	-1.0000E-02

100 ITERATIONS IN CCFR AT POINT   1
100 ITERATIONS IN CCFR AT POINT   1
ITERATION 1 SIGMA= 194.96603   SUM OF SQUARES = 2.1287E+06

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	1.0000E -2	-.4487	5.5130E -3	2.6973
BETA B	4.6774E 10	-.9000	4.6774E 9	4.8810
BETA C	.6310E-18	-.2832	4.5230E-19	2.6546
BETA G	.1698E-13	.5156	2.5738E-14	.7314

ITERATION 2 SIGMA= 167.53638   SUM OF SQUARES = 1.5718E+06

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	5.5130E -3	-.5327	2.5761E -3	2.2818
BETA B	4.6774E 9	-.9000	4.6774E 8	4.4480
BETA C	4.5230E-19	-.3552	2.9166E-19	2.2678
BETA G	2.5738E-14	.7218	4.4317E-14	.6830

ITERATION 3 SIGMA= 135.22029   SUM OF SQUARES = 1.0239E+06

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	2.5761E -3	-.7332	6.8740E -4	1.9177
BETA B	4.6774E 8	-.9000	4.6774E 7	4.4924
BETA C	2.9166E-19	-.5376	1.3485E-19	1.8659
BETA G	4.4317E-14	1.3173	1.0270E-13	.6321

ITERATION 4 SIGMA= 89.76459 SUM OF SQUARES = 4.5123E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.8740E -4	-.0201	6.7358E -4	1.4786
BETA B	4.6774E 7	.6647	7.7862E 7	4.7105
BETA C	1.3485E-19	-.1955	1.0849E-19	1.3186
BETA G	1.0270E-13	1.7653	2.8398E-13	.5535

ITERATION 5 SIGMA= 45.40074 SUM OF SQUARES = 1.1543E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.7358E -4	.4062	9.4720E -4	.8214
BETA B	7.7862E 7	.2169	9.4754E 7	2.1126
BETA C	1.0849E-19	.4041	1.5233E-19	.8993
BETA G	2.8398E-13	1.4055	6.8311E-13	.5019

ITERATION 6 SIGMA= 21.90980 SUM OF SQUARES = 2.6882E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	9.4720E -4	1.0248	1.9179E -3	.5139
BETA B	9.4754E 7	.8104	1.7154E 8	1.1382
BETA C	1.5233E-19	1.3975	3.6521E-19	.6604
BETA G	6.8311E-13	1.2686	1.5497E-12	.3308

ITERATION 7 SIGMA= 14.42713 SUM OF SQUARES = 1.1656E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	1.9179E -3	.6626	3.1886E -3	.4762
BETA B	1.7154E 8	.4901	2.5562E 8	.8448
BETA C	3.6521E-19	1.0966	7.6569E-19	.6653
BETA G	1.5497E-12	.3938	2.1599E-12	.2301

ITERATION 8 SIGMA= 8.51962 SUM OF SQUARES = 4.0647E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	3.1886E -3	.4060	4.4834E -3	.3133
BETA B	2.5562E 8	.3979	3.5733E 8	.5232
BETA C	7.6569E-19	.8239	1.3966E-18	.4576
BETA G	2.1599E-12	.1654	2.5172E-12	.1365

ITERATION 9 SIGMA= 5.73476 SUM OF SQUARES = 1.8417E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	4.4834E -3	.1880	5.3264E -3	.2045
BETA B	3.5733E 8	.2547	4.4833E 8	.3565

BETA C	1.3966E-18	.4640	2.0446E-18	.3012
BETA G	2.5172E-12	.0690	2.6910E-12	.0820

ITERATION 10 SIGMA= 4.24593 SUM OF SQUARES = 1.0096E+03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	5.3264E -3	.1295	6.0160E -3	.1438
BETA B	4.4833E 8	.1599	5.2002E 8	.2622
BETA C	2.0446E-18	.2900	2.6376E-18	.2096
BETA G	2.6910E-12	.0550	2.8390E-12	.0542

ITERATION 11 SIGMA= 3.97643 SUM OF SQUARES = 8.8547E+02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.0160E -3	-.0088	5.9628E -3	.1318
BETA B	5.2002E 8	.0375	5.3953E 8	.2460
BETA C	2.6376E-18	.0131	2.6720E-18	.1912
BETA G	2.8390E-12	-.0060	2.8220E-12	.0474

ITERATION 12 SIGMA= 3.93164 SUM OF SQUARES = 8.6564E+02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	5.9628E -3	.0033	5.9825E -3	.1290
BETA B	5.3953E 8	.0003	5.3969E 8	.2405
BETA C	2.6720E-18	.0066	2.6897E-18	.1858
BETA G	2.8220E-12	.0019	2.8273E-12	.0462

1 GETHITE- Zn IN 0.100 M NANO3 <1:1:1> for metal
CHI-SQUARED = 4.70
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
SIGMA = 3.9316

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION			
BETA A REFINED	5.98246E -3	.1290	-2.22312	.05996	1	1	-1
BETA B REFINED	5.39693E 8	.2405	8.73215	.11947	1	2	0
BETA C REFINED	2.68971E-18	.1858	-17.57030	.08926	1	1	-3
BETA D CONSTANT	.79433E-17		-17.10000		1	0	-2
BETA E CONSTANT	.16596E -9		-9.78000		0	1	-1
BETA F CONSTANT	6.45654E 6		6.81000		0	1	1
BETA G REFINED	2.82733E-12	.0462	-11.54862	.02053	0	0	-1

ITERATION 1 SIGMA= 3.75599 SUM OF SQUARES = 7.9002E+02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	5.9825E -3	.0766	6.4409E -3	.1184
BETA B	5.3969E 8	.1438	6.1729E 8	.2150
BETA C	2.6897E-18	.0877	2.9256E-18	.1689
BETA G	2.8273E-12	.0054	2.8426E-12	.0428

CURVE 1 ADDED CONC Hydrogen -1.6203E-02 .0218 -1.6238E-02 .1751

ITERATION 2 SIGMA= 3.72878 SUM OF SQUARES = 7.7861E+02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	6.4409E -3	.0027	6.4581E -3	.1176
BETA B	6.1729E 8	.0107	6.2388E 8	.2098
BETA C	2.9256E-18	.0044	2.9384E-18	.1676
BETA G	2.8426E-12	.0002	2.8433E-12	.0421

CURVE 1 ADDED CONC Hydrogen -1.6238E-02   .0009 -1.6240E-02   .1724
1 GETHITE- Zn IN 0.100 M NANO3 <1:1:1> for metal
  2 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY

	CLASS LIMITS		PROBABILITY		FREQUENCY		PARTIAL
	LOWER	HIGHER	CALC	OBS	CALC	OBS	CHI-SQUARE
1	-.10000E+76	-.42881E+01	.1250	.1639	7.6	10	.740
2	-.42881E+01	-.25169E+01	.1250	.0820	7.6	5	.904
3	-.25169E+01	-.11895E+01	.1250	.1148	7.6	7	.051
4	-.11895E+01	.00000E+00	.1250	.1311	7.6	8	.018
5	.00000E+00	.11895E+01	.1250	.0656	7.6	4	1.723
6	.11895E+01	.25169E+01	.1250	.1639	7.6	10	.740
7	.25169E+01	.42881E+01	.1250	.1311	7.6	8	.018
8	.42881E+01	.10000E+76	.1250	.1475	7.6	9	.248

CHI-SQUARED = **4.44**
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
  SIGMA =   3.7288

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION			
BETA A REFINED	6.45810E -3	.1176	**-2.18990**	.05434	1	1	-1
BETA B REFINED	6.23878E 8	.2098	**8.79510**	.10226	1	2	0
BETA C REFINED	2.93837E-18	.1676	**-17.53189**	.07967	1	1	-3
BETA D CONSTANT	.79433E-17		-17.10000		1	0	-2
BETA E CONSTANT	.16596E -9		-9.78000		0	1	-1
BETA F CONSTANT	6.45654E 6		6.81000		0	1	1
BETA G REFINED	2.84326E-12	.0421	-11.54618	.01868	0	0	-1

4. The system of Goethite($\equiv$FeOH) - H$^+$- Cu^{2+}- SO$_4$$^{2-}$

MAXIT	IPRIN	MODE	TOL	ACCM	RELAC
99	5	2	.10E-03	.10E-74	.601347-153

REACTANT 1- CU
REACTANT 2- GOETHTE
REACTANT 3- SULPHATE
REACTANT 4- Hydrogen
THE TEMPERATURE OF SOLUTION(S) IS 25.00 DEGREES CENTIGRADE

	FORMATION CONSTANTS	LOG BETAS	REFINEMENT KEYS	STOICHIOMETRIC COEFFICIENTS			
A	5.2481E 13	13.7200	0	1	1	1	0
B	8.9125E 8	8.9500	0	1	1	1	-1
C	5.6234E 1	1.7500	1	1	1	1	-2
D	.7586E -8	-8.1200	0	1	0	0	-1
E	2.0417E 6	6.3100	0	1	1	0	0
F	7.9433E 0	.9000	0	1	1	0	-1
G	.4898E -9	-9.3100	0	1	1	0	-2
H	1.9953E 8	8.3000	0	0	1	1	1
I	3.1623E 13	13.5000	0	0	1	1	2
J	.1660E -9	-9.7800	0	0	1	0	-1
K	6.4565E 6	6.8100	0	0	1	0	1
L	.1698E-13	-13.7700	0	0	0	0	-1

1 FORMATION CONSTANTS TO BE REFINED
2 SPECIAL PARAMETERS TO BE REFINED

		CURVE	VALUE
TOT MMOLES	CU	1	1.0000E-02
TOT MMOLES	SULPHATE	1	1.0000E-02

1 GTHITE-Cu-SO4 IN 0.100 M NANO3 <1:1:1> for metal
10 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY
CHI-SQUARED = 5.49
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
SIGMA = 16.6675

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION				
BETA A CONSTANT	5.24807E 13		13.72000		1	1	1	0
BETA B CONSTANT	8.91251E 8		8.95000		1	1	1	-1
BETA C REFINED	5.15157E 1	.1175	1.71194	.05427	1	1	1	-2
BETA D CONSTANT	.75858E -8		-8.12000		1	0	0	-1
BETA E CONSTANT	2.04174E 6		6.31000		1	1	0	0
BETA F CONSTANT	7.94328E 0		.90000		1	1	0	-1
BETA G CONSTANT	.48978E -9		-9.31000		1	1	0	-2
BETA H CONSTANT	1.99526E 8		8.30000		0	1	1	1
BETA I CONSTANT	3.16228E 13		13.50000		0	1	1	2

BETA J CONSTANT   .16596E -9   -9.78000   0 1 0 -1
BETA K CONSTANT 6.45654E 6   6.81000   0 1 0 1
BETA L CONSTANT .16982E-13   -13.77000   0 0 0 -1

	CURVE	INITIAL VALUE	FINAL VALUE	STD DEV
TOT MMOLES CU	1	.01000	.01178	.00025
TOT MMOLES SULPHATE	1	.01000	.00957	.00003

ITERATION 1 SIGMA= 338.11932   SUM OF SQUARES = 6.6308E+06
MARQUART PARAMETER FOR NEXT ITERATION 1.7895E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.0000E 2	-.9000	10.0000E 0	31.8824

ITERATION 2 SIGMA= 323.07468   SUM OF SQUARES = 6.0539E+06
MARQUART PARAMETER FOR NEXT ITERATION 1.7895E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	10.0000E 0	.4624	1.4624E 1	8.5874

ITERATION 3 SIGMA= 186.72833   SUM OF SQUARES = 2.0223E+06
MARQUART PARAMETER FOR NEXT ITERATION 8.9474E-03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.4624E 1	2.3071	4.8364E 1	.9597

ITERATION 4 SIGMA= 77.24629   SUM OF SQUARES = 3.4609E+05
MARQUART PARAMETER FOR NEXT ITERATION 4.4737E-03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	4.8364E 1	1.4839	1.2013E 2	.3087

ITERATION 5 SIGMA= 44.09600   SUM OF SQUARES = 1.1278E+05
MARQUART PARAMETER FOR NEXT ITERATION 2.2369E-03

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.2013E 2	.5765	1.8939E 2	.1706

ITERATION 6 SIGMA= 31.85779   SUM OF SQUARES = 5.8865E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.8939E 2	.1244	2.1295E 2	.1206

ITERATION 7 SIGMA= 31.14489   SUM OF SQUARES = 5.6260E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	2.1295E 2	.0066	2.1437E 2	.1172

ITERATION 8 SIGMA= 31.13721   SUM OF SQUARES = 5.6232E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	2.1437E 2	-.0003	2.1431E 2	.1171

ITERATION 9 SIGMA= 31.13484   SUM OF SQUARES = 5.6224E+04

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	2.1431E 2	-.0002	2.1425E 2	.1170

1 GOETHITE-Cu-SO4 IN 0.500 M NANO3 <1:1:1> for metal
 9 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY
 CHI-SQUARED = 2.08
 CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
 SIGMA = 31.1348

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION				
BETA A CONSTANT	1.00000E 11		11.00000		1	1	1	0
BETA B CONSTANT	1.00000E 6		6.00000		1	1	1	-1
BETA C REFINED	2.14254E 2	.1170	2.33093	.05406	1	1	1	-2
BETA D CONSTANT	.75858E -8		-8.12000		1	0	0	-1
BETA E CONSTANT	7.41310E 4		4.87000		1	1	0	0
BETA F CONSTANT	7.94328E 0		.90000		1	1	0	-1
BETA G CONSTANT	.25119E -6		-6.60000		1	1	0	-2
BETA H CONSTANT	1.99526E 8		8.30000		0	1	1	1
BETA I CONSTANT	3.16228E 13		13.50000		0	1	1	2
BETA J CONSTANT	.11220E -8		-8.95000		0	1	0	-1
BETA K CONSTANT	2.04174E 6		6.31000		0	1	0	1
BETA L CONSTANT	.12303E-12		-12.91000		0	0	0	-1

CORRELATION MATRIX - PARAMETERS ORDERED AS ABOVE
   1   2
   2   2 .73
 3 .28 .56
REFINEMENT CONTINUES WITH WEIGHTS OBTAINED FROM THE
CALCULATED TITRATION CURVES1
ITERATION 1 SIGMA= 126.62695   SUM OF SQUARES = 9.2999E+05
MARQUART PARAMETER FOR NEXT ITERATION 7.4481E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	2.1425E 2	-.0643	2.0048E 2	.2369

ITERATION 2 SIGMA= 98.31595   SUM OF SQUARES = 5.6063E+05
MARQUART PARAMETER FOR NEXT ITERATION 3.7240E-02

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	2.0048E 2	-.0087	1.9873E 2	.1500

ITERATION 3 SIGMA= 85.71273   SUM OF SQUARES = 4.2611E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.9873E 2	-.0823	1.8239E 2	.1294

ITERATION 4 SIGMA= 84.27311   SUM OF SQUARES = 4.1191E+05

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA C	1.8239E 2	-.0786	1.6806E 2	.1265

ITERATION 5 SIGMA= 83.83071   SUM OF SQUARES = 4.0760E+05
     PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
       BETA C   1.6806E 2   .0140   1.7041E 2   .1257

ITERATION 6 SIGMA= 83.79750   SUM OF SQUARES = 4.0728E+05
     PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
       BETA C   1.7041E 2   -.0051   1.6955E 2   .1251

4 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY
  CHI-SQUARED = 3.92
  CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
  SIGMA =   24.8147

	VALUE	REL STD DEV	LOG BETA	STD	DEVIATION
BETA A CONSTANT	5.24807E 13		13.72000		1 1 1 0
BETA B CONSTANT	8.91251E 8		8.95000		1 1 1 -1
BETA C REFINED	4.76009E 1	.1244	**1.67762**	.05771	1 1 1 -2
BETA D CONSTANT	.75858E -8		-8.12000		1 0 0 -1
BETA E CONSTANT	2.04174E 6		6.31000		1 1 0 0
BETA F CONSTANT	7.94328E 0		.90000		1 1 0 -1
BETA G CONSTANT	.48978E -9		-9.31000		1 1 0 -2
BETA H CONSTANT	1.99526E 8		8.30000		0 1 1 1
BETA I CONSTANT	3.16228E 13		13.50000		0 1 1 2
BETA J CONSTANT	.16596E -9		-9.78000		0 1 0 -1
BETA K CONSTANT	6.45654E 6		6.81000		0 1 0 1
BETA L CONSTANT	.16982E-13		-13.77000		0 0 0 -1

5. The system of goethite($\equiv$FeOH) - H^+- Zn^{2+}- SO_4^{2-}

MAXIT	IPRIN	MODE	TOL	ACCM	RELAC
99	5	2	.10E-03	.10E-74	.601347-153

REACTANT 1- zn
REACTANT 2- GOETHTE
REACTANT 3- SULPHATE
REACTANT 4- Hydrogen
THE TEMPERATURE OF SOLUTION(S) IS 25.00 DEGREES CENTIGRADE

	FORMATION CONSTANTS	LOG BETAS	REFINEMENT KEYS	STOICHIOMETRIC COEFFICIENTS			
A	7.2444E 13	13.8600	1	1	1	1	-1
B	3.1623E 19	19.5000	0	1	2	1	0
C	.2884E -2	-2.5400	0	1	1	1	-3
D	.7943E-17	-17.1000	0	1	0	0	-2
E	.6457E -2	-2.1900	0	1	1	0	-1
F	6.3096E 8	8.8000	0	1	2	0	0
G	.2951E-17	-17.5300	0	1	1	0	-3
H	1.9953E 8	8.3000	0	0	1	1	1
I	3.1623E 13	13.5000	0	0	1	1	2
J	.1660E -9	-9.7800	0	0	1	0	-1
K	6.4565E 6	6.8100	0	0	1	0	1
L	.1698E-13	-13.7700	0	0	0	0	-1

1 FORMATION CONSTANTS TO BE REFINED
CURVE 1 INITIAL VOLUME 33.00
TITRE VOLUME ERROR .01000 MILLILITRES

REACTANT	INITIAL NO OF MILLIMOLES	TITRANT MOLES/LITRE	STANDARD POTENTIAL MILLIVOLTS	ELECTRODE ERROR
zn	.01000	.00000		NO ELECTRODE
GOETHTE	.01000	.00000		NO ELECTRODE
SULPHATE	.01000	.00000	441.60000	.05000
Hydrogen	.01000	-.01000		NO ELECTRODE

2 SPECIAL PARAMETERS TO BE REFINED

ITERATION 1 SIGMA= 422.91578 SUM OF SQUARES = 1.0374E+07

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	7.2444E 13	6.2289	5.2369E 14	2.8887

ITERATION 2 SIGMA= 143.52320 SUM OF SQUARES = 1.1947E+06

PARAMETER	OLD VALUE	REL SHIFT	NEW VALUE	REL ERROR
BETA A	5.2369E 14	-.9000	5.2369E 13	1.2582

ITERATION 3 SIGMA= 114.62380 SUM OF SQUARES = 7.6204E+05

PARAMETER OLD VALUE REL SHIFT NEW VALUE REL ERROR

BETA A   5.2369E 13   .3820   7.2372E 13   .4971

ITERATION   4   SIGMA= 69.26700   SUM OF SQUARES = 2.7828E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   7.2372E 13   -.0022   7.2212E 13   .3763

ITERATION   5   SIGMA= 62.93245   SUM OF SQUARES = 2.2971E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   7.2212E 13   -.0397   6.9345E 13   .3581

ITERATION   6   SIGMA= 62.87324   SUM OF SQUARES = 2.2928E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   6.9345E 13   -.0722   6.4336E 13   .3618

ITERATION   7   SIGMA= 62.29781   SUM OF SQUARES = 2.2510E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   6.4336E 13   -.3056   4.4673E 13   .3595

ITERATION   8   SIGMA= 57.53508   SUM OF SQUARES = 1.9200E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   4.4673E 13   -.4226   2.5793E 13   .3319

ITERATION   9   SIGMA= 54.24609   SUM OF SQUARES = 1.7067E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   2.5793E 13   -.1396   2.2192E 13   .2733

ITERATION 10   SIGMA= 51.31138   SUM OF SQUARES = 1.5271E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   2.2192E 13   -.2537   1.6563E 13   .2549

ITERATION 11   SIGMA= 49.21502   SUM OF SQUARES = 1.4048E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   1.6563E 13   -.2247   1.2842E 13   .2591

ITERATION 12   SIGMA= 46.62201   SUM OF SQUARES = 1.2607E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   1.2842E 13   -.2268   9.9286E 12   .2468

ITERATION 13   SIGMA= 44.40298   SUM OF SQUARES = 1.1435E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   9.9286E 12   -.1956   7.9864E 12   .2444

ITERATION 14   SIGMA= 42.53979   SUM OF SQUARES = 1.0496E+05
     PARAMETER   OLD VALUE   REL SHIFT   NEW VALUE   REL ERROR
     BETA A   7.9864E 12   -.1428   6.8459E 12   .2446

ITERATION 15 SIGMA= 41.14182   SUM OF SQUARES = 9.8174E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　6.8459E 12   -.0116   6.7662E 12   .1979

ITERATION 16 SIGMA= 40.95849   SUM OF SQUARES = 9.7301E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　6.7662E 12   -.0144   6.6687E 12   .2038

ITERATION 17 SIGMA= 40.93678   SUM OF SQUARES = 9.7198E+04

　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　6.6687E 12   -.0164   6.5590E 12   .2111

ITERATION 18 SIGMA= 40.90452   SUM OF SQUARES = 9.7044E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　6.5590E 12   -.0365   6.3193E 12   .2227

ITERATION 19 SIGMA= 40.79973   SUM OF SQUARES = 9.6548E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　6.3193E 12   -.0977   5.7018E 12   .2385

ITERATION 20 SIGMA= 40.26227   SUM OF SQUARES = 9.4021E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　5.7018E 12   -.1370   4.9205E 12   .2281

ITERATION 21 SIGMA= 39.30643   SUM OF SQUARES = 8.9610E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　4.9205E 12   -.0829   4.5123E 12   .2375

ITERATION 22 SIGMA= 38.92139   SUM OF SQUARES = 8.7863E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　4.5123E 12   -.1321   3.9164E 12   .2350

ITERATION 23 SIGMA= 38.09944   SUM OF SQUARES = 8.4191E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　3.9164E 12   -.0178   3.8467E 12   .2225

ITERATION 24 SIGMA= 38.04244   SUM OF SQUARES = 8.3939E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　3.8467E 12   -.0653   3.5955E 12   .2367

ITERATION 25 SIGMA= 37.82929   SUM OF SQUARES = 8.3001E+04
　　PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
　　BETA A　　　　　3.5955E 12   -.1088   3.2044E 12   .2418

ITERATION 26 SIGMA= 37.32548   SUM OF SQUARES = 8.0805E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   3.2044E 12   -.0486   3.0487E 12   .2216

ITERATION 27 SIGMA= 37.10424   SUM OF SQUARES = 7.9850E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   3.0487E 12   -.0106   3.0162E 12   .2234

ITERATION 28 SIGMA= 37.09353   SUM OF SQUARES = 7.9804E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   3.0162E 12   -.0201   2.9555E 12   .2309

ITERATION 29 SIGMA= 37.06542   SUM OF SQUARES = 7.9683E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.9555E 12   -.0436   2.8266E 12   .2413

ITERATION 30 SIGMA= 36.96515   SUM OF SQUARES = 7.9252E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.8266E 12   -.0807   2.5985E 12   .2480

ITERATION 31 SIGMA= 36.71743   SUM OF SQUARES = 7.8194E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.5985E 12   -.0604   2.4416E 12   .2402

ITERATION 32 SIGMA= 36.53029   SUM OF SQUARES = 7.7399E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.4416E 12   -.0240   2.3831E 12   .2297

ITERATION 33 SIGMA= 36.45555   SUM OF SQUARES = 7.7082E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.3831E 12   -.0033   2.3752E 12   .2227

ITERATION 34 SIGMA= 36.45170   SUM OF SQUARES = 7.7066E+04
  PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
   BETA A   2.3752E 12   -.0024   2.3696E 12   .2238
  34 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY
 CHI-SQUARED = 6.54
 CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
 SIGMA = 36.4517

	VALUE	REL STD DEV	LOG BETA	STD DEVIATION				
BETA A REFINED	2.36961E 12	.2238	12.37468	.11002	1	1	1	-1
BETA B CONSTANT	3.16228E 19		19.50000		1	2	1	0
BETA C CONSTANT	.28840E -2		-2.54000		1	1	1	-3
BETA D CONSTANT	.79433E-17		-17.10000		1	0	0	-2

BETA E CONSTANT   .64565E -2   -2.19000   1 1 0 -1
BETA F CONSTANT 6.30957E 8   8.80000   1 2 0 0
BETA G CONSTANT   .29512E-17   - 17.53000   1 1 0 -3
BETA H CONSTANT 1.99526E 8   8.30000   0 1 1 1
BETA I CONSTANT 3.16228E 13   13.50000   0 1 1 2
BETA J CONSTANT   .16596E -9   -9.78000   0 1 0 -1
BETA K CONSTANT 6.45654E 6   6.81000   0 1 0 1
BETA L CONSTANT   .16982E-13   -13.77000   0 0 0 -1
                    CURVE INITIAL VALUE   FINAL VALUE   STD DEV
TOT MMOLES   SULPHATE   1   .01000   .01000   .00000
TOT MMOLES   Hydrogen   1   .01000   -.00473   -.00018
CORRELATION MATRIX - PARAMETERS ORDERED AS ABOVE
   1   2
2 .20
3 -.32 .05
REFINEMENT CONTINUES WITH WEIGHTS OBTAINED FROM THE
CALCULATED TITRATION CURVES1
ITERATION 1 SIGMA= 110.67163   SUM OF SQUARES = 7.1040E+05
MARQUART PARAMETER FOR NEXT ITERATION 3.6271E-01
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   2.3696E 12   .0683 2.5314E 12   .6433

ITERATION 2 SIGMA= 101.24425   SUM OF SQUARES = 5.9452E+05
MARQUART PARAMETER FOR NEXT ITERATION 1.8135E-01
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   2.5314E 12   .1293 2.8586E 12   .3784

ITERATION 3 SIGMA= 100.09075   SUM OF SQUARES = 5.8105E+05
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   2.8586E 12   .1077 3.1664E 12   .3768

ITERATION 4 SIGMA= 99.54688   SUM OF SQUARES = 5.7476E+05
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   3.1664E 12   .1420 3.6159E 12   .3753

ITERATION 5 SIGMA= 98.70802   SUM OF SQUARES = 5.6511E+05
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   3.6159E 12   .1405 4.1239E 12   .3520

ITERATION 6 SIGMA= 98.02717   SUM OF SQUARES = 5.5734E+05
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   4.1239E 12   .0302 4.2485E 12   .3282

ITERATION 7 SIGMA= 97.94672   SUM OF SQUARES = 5.5643E+05
      PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
      BETA A   4.2485E 12   .0310 4.3803E 12   .3297

ITERATION 8 SIGMA= 97.87189   SUM OF SQUARES = 5.5558E+05
    PARAMETE OLD VALUE   REL SHIFT NEW VALUE REL ERROR
     BETA A   4.3803E 12   .0319   4.5202E 12   .3307

ITERATION 9 SIGMA= 97.80920   SUM OF SQUARES = 5.5487E+05
    PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
     BETA A   4.5202E 12   .0325   4.6670E 12   .3313

ITERATION 10 SIGMA= 97.75187   SUM OF SQUARES = 5.5421E+05
    PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
     BETA A   4.6670E 12   .0351   4.8308E 12   .3313

ITERATION 11 SIGMA= 97.68816   SUM OF SQUARES = 5.5349E+05
    PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
     BETA A   4.8308E 12   .0416   5.0318E 12   .3303

ITERATION 12 SIGMA= 97.59852   SUM OF SQUARES = 5.5248E+05
    PARAMETER OLD VALUE   REL SHIFT NEW VALUE REL ERROR
     BETA A   5.0318E 12   .0538   5.3028E 12   .3274
  16 ITERATIONS
REFINEMENT TERMINATED SUCCESSFULLY
  CHI-SQUARED = 7.59
CHI SQUARED SHOULD BE LESS THAN 12.60 AT THE 95 PERCENT
CONFIDENCE LEVEL
  SIGMA = 97.0575

	VALUE	REL STD DEV	LOG BETA	STD	DEVIATION			
BETA A REFINED	5.87664E 12	.2678	**12.63913**	.13539	1	1	1	-1
BETA B CONSTANT	3.16228E 19		19.50000		1	2	1	0
BETA C CONSTANT	.28840E -2		-2.54000		1	1	1	-3
BETA D CONSTANT	.79433E-17		-17.10000		1	0	0	-2
BETA E CONSTANT	.64565E -2		-2.19000		1	1	0	-1
BETA F CONSTANT	6.30957E 8		8.80000		1	2	0	0
BETA G CONSTANT	.29512E-17		-17.53000		1	1	0	-3
BETA H CONSTANT	1.99526E 8		8.30000		0	1	1	1
BETA I CONSTANT	3.16228E 13		13.50000		0	1	1	2
BETA J CONSTANT	.16596E -9		-9.78000		0	1	0	-1
BETA K CONSTANT	6.45654E 6		6.81000		0	1	0	1
BETA L CONSTANT	.16982E-13		-13.77000		0	0	0	-1

APPENDIX F

Determination of the surface charge density, σ_0

0.500 M NaNO$_3$

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-'OH^-])]$ x96485/302.72 surface charge density (δ_0)
0	4.608	0.000303	0	2.46604E-05	4.05509E-10	0.00027837	26.85848	0.088724
0.08	4.812	0.000302	2.42E-05	1.5417E-05	6.48634E-10	0.0002627	25.34622	0.083728
0.16	5.037	0.000302	4.83E-05	9.18333E-06	1.08893E-09	0.00024413	23.55516	0.077812
0.24	5.267	0.000301	7.22E-05	5.40754E-06	1.84927E-09	0.00022323	21.53842	0.07115
0.32	5.492	0.0003	9.6E-05	3.22107E-06	3.10456E-09	0.00020086	19.37973	0.064019
0.4	5.707	0.000299	0.00012	1.96336E-06	5.09331E-09	0.00017767	17.14271	0.056629
0.48	5.911	0.000299	0.000143	1.22744E-06	8.14704E-09	0.00015408	14.86651	0.04911
0.56	6.107	0.000298	0.000167	7.81628E-07	1.27938E-08	0.00013031	12.57335	0.041535
0.64	6.291	0.000297	0.00019	5.11682E-07	1.95434E-08	0.00010648	10.27413	0.033939
0.72	6.467	0.000297	0.000214	3.41193E-07	2.93089E-08	8.2666E-05	7.976055	0.026348
0.8	6.633	0.000296	0.000237	2.32809E-07	4.29536E-08	5.8896E-05	5.682565	0.018772
0.88	6.795	0.000295	0.00026	1.60325E-07	6.23735E-08	3.5196E-05	3.395927	0.011218
0.96	6.954	0.000294	0.000283	1.11173E-07	8.99498E-08	1.1577E-05	1.117049	0.00369
1.04	7.108	0.000294	0.000306	7.7983E-08	1.28233E-07	-1.196E-05	-1.15368	-0.00381
1.12	7.262	0.000293	0.000328	5.47016E-08	1.8281E-07	-3.541E-05	-3.41629	-0.01129
1.2	7.411	0.000292	0.000351	3.8815E-08	2.57632E-07	-5.878E-05	-5.671	-0.01873
1.28	7.559	0.000292	0.000373	2.76058E-08	3.62243E-07	-8.207E-05	-7.91854	-0.02616
1.36	7.708	0.000291	0.000396	1.95884E-08	5.10505E-07	-0.0001053	-10.1602	-0.03356
1.44	7.845	0.00029	0.000418	1.42889E-08	6.99842E-07	-0.0001285	-12.3957	-0.04095
1.52	7.978	0.00029	0.00044	1.05196E-08	9.50605E-07	-0.0001516	-14.627	-0.04832
1.6	8.093	0.000289	0.000462	8.07235E-09	1.2388E-06	-0.0001747	-16.8518	-0.05567
1.68	8.205	0.000288	0.000484	6.23735E-09	1.60325E-06	-0.0001977	-19.0739	-0.06301
1.76	8.305	0.000288	0.000506	4.9545E-09	2.01837E-06	-0.0002207	-21.2909	-0.07033
1.84	8.394	0.000287	0.000528	4.03645E-09	2.47742E-06	-0.0002436	-23.5022	-0.07764

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A - C_B - [H^+] - [OH^-])]$	$[(C_A - C_B - [H^+] - [OH^-])]$ x96485	$[(C_A - C_B - [H^+] - [OH^-])]$ x96485/302.72 surface charge density (δ_0)
1.92	8.474	0.000286	0.00055	3.35738E-09	2.97852E-06	-0.0002664	-25.7076	-0.08492
2	8.545	0.000286	0.000571	2.85102E-09	3.50752E-06	-0.0002892	-27.9058	-0.09218
2.08	8.609	0.000285	0.000593	2.46037E-09	4.06443E-06	-0.0003119	-30.097	-0.09942
2.16	8.666	0.000284	0.000614	2.15774E-09	4.63447E-06	-0.0003346	-32.2797	-0.10663
2.24	8.719	0.000284	0.000636	1.90985E-09	5.236E-06	-0.0003571	-34.4558	-0.11382
2.32	8.765	0.000283	0.000657	1.71791E-09	5.82103E-06	-0.0003795	-36.6208	-0.12097
2.4	8.807	0.000282	0.000678	1.55955E-09	6.4121E-06	-0.0004019	-38.7767	-0.12809
2.48	8.847	0.000282	0.000699	1.42233E-09	7.03072E-06	-0.0004242	-40.9259	-0.13519
2.56	8.885	0.000281	0.00072	1.30317E-09	7.67361E-06	-0.0004464	-43.068	-0.14227
2.64	8.918	0.000281	0.000741	1.20781E-09	8.27942E-06	-0.0004684	-45.1972	-0.1493
2.72	8.954	0.00028	0.000761	1.11173E-09	8.99498E-06	-0.0004905	-47.3277	-0.15634
2.8	8.984	0.000279	0.000782	1.03753E-09	9.63829E-06	-0.0005124	-49.4421	-0.16333
2.88	9.01	0.000279	0.000803	9.77237E-10	1.02329E-05	-0.0005342	-51.5425	-0.17026
2.96	9.035	0.000278	0.000823	9.22571E-10	1.08393E-05	-0.0005559	-53.6351	-0.17718
3.04	9.057	0.000277	0.000844	8.77001E-10	1.14025E-05	-0.0005774	-55.7144	-0.18405
3.12	9.081	0.000277	0.000864	8.29851E-10	1.20504E-05	-0.000599	-57.7929	-0.19091
3.2	9.101	0.000276	0.000884	7.92501E-10	1.26183E-05	-0.0006204	-59.8548	-0.19772
3.28	9.125	0.000276	0.000904	7.49894E-10	1.33352E-05	-0.0006418	-61.9223	-0.20455
3.36	9.147	0.000275	0.000924	7.12853E-10	1.40281E-05	-0.0006631	-63.9786	-0.21135
3.44	9.169	0.000274	0.000944	6.77642E-10	1.47571E-05	-0.0006844	-66.0297	-0.21812
3.52	9.192	0.000274	0.000964	6.42688E-10	1.55597E-05	-0.0007056	-68.0792	-0.22489
3.6	9.211	0.000273	0.000984	6.15177E-10	1.62555E-05	-0.0007266	-70.1097	-0.2316
3.68	9.229	0.000273	0.001003	5.90201E-10	1.69434E-05	-0.0007476	-72.131	-0.23828
3.76	9.245	0.000272	0.001023	5.68853E-10	1.75792E-05	-0.0007684	-74.1387	-0.24491
3.84	9.261	0.000271	0.001042	5.48277E-10	1.8239E-05	-0.0007891	-76.1402	-0.25152
3.92	9.277	0.000271	0.001062	5.28445E-10	1.89234E-05	-0.0008098	-78.1358	-0.25811
4	9.29	0.00027	0.001081	5.12861E-10	1.94984E-05	-0.0008303	-80.1124	-0.26464

0.100 M NaNO₃

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (6_0)
0	4.099	0.000323	0	7.96159E-05	1.25603E-10	0.000242965	23.44244	0.077439
0.07	4.267	0.000322	2.25E-05	5.40754E-05	1.84927E-10	0.000245248	23.6628	0.078167
0.14	4.483	0.000321	4.5E-05	3.28852E-05	3.04089E-10	0.000243287	23.47351	0.077542
0.21	4.731	0.00032	6.73E-05	1.8578E-05	5.3827E-10	0.000234545	22.63011	0.074756
0.28	4.995	0.00032	8.95E-05	1.01158E-05	9.88553E-10	0.000220062	21.23271	0.07014
0.35	5.267	0.000319	0.000112	5.40754E-06	1.84927E-09	0.000201927	19.48294	0.06436
0.42	5.529	0.000318	0.000134	2.95801E-06	3.38065E-09	0.000181634	17.525	0.057892
0.49	5.773	0.000318	0.000156	1.68655E-06	5.92925E-09	0.000160264	15.46304	0.05108
0.56	5.999	0.000317	0.000177	1.00231E-06	9.977E-09	0.000138405	13.35398	0.044113
0.63	6.216	0.000316	0.000199	6.08135E-07	1.64437E-08	0.000116353	11.22632	0.037085
0.7	6.42	0.000315	0.000221	3.80189E-07	2.63027E-08	9.42307E-05	9.091852	0.030034
0.77	6.62	0.000315	0.000242	2.39883E-07	4.16869E-08	7.21138E-05	6.957897	0.022985
0.84	6.807	0.000314	0.000264	1.55955E-07	6.4121E-08	5.00312E-05	4.827258	0.015946
0.91	6.997	0.000313	0.000285	1.00693E-07	9.93116E-08	2.80043E-05	2.701997	0.008926
0.98	7.181	0.000313	0.000306	6.59174E-08	1.51705E-07	6.03629E-06	0.582411	0.001924
1.05	7.36	0.000312	0.000328	4.36516E-08	2.29087E-07	-1.5873E-05	-1.53154	-0.00506
1.12	7.543	0.000311	0.000349	2.86418E-08	3.4914E-07	-3.7738E-05	-3.64112	-0.01203
1.19	7.715	0.000311	0.00037	1.92752E-08	5.188E-07	-5.9563E-05	-5.7469	-0.01898
1.26	7.879	0.00031	0.000391	1.3213E-08	7.56833E-07	-8.1365E-05	-7.85052	-0.02593
1.33	8.036	0.000309	0.000411	9.2045E-09	1.08643E-06	-0.00010317	-9.95417	-0.03288
1.4	8.178	0.000309	0.000432	6.63743E-09	1.50661E-06	-0.00012497	-12.0577	-0.03983
1.47	8.307	0.000308	0.000453	4.93174E-09	2.02768E-06	-0.00014678	-14.1622	-0.04678
1.54	8.42	0.000307	0.000473	3.80189E-09	2.63027E-06	-0.00016858	-16.2658	-0.05373
1.61	8.518	0.000307	0.000494	3.03389E-09	3.2961E-06	-0.00019036	-18.3667	-0.06067
1.68	8.604	0.000306	0.000514	2.48886E-09	4.01791E-06	-0.0002121	-20.4643	-0.0676
1.75	8.682	0.000305	0.000534	2.0797E-09	4.80839E-06	-0.00023382	-22.5599	-0.07452

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (δ_0)
1.82	8.748	0.000305	0.000555	1.78649E-09	5.59758E-06	-0.00025545	-24.6468	-0.08142
1.89	8.805	0.000304	0.000575	1.56675E-09	6.38263E-06	-0.00027698	-26.7247	-0.08828
1.96	8.856	0.000303	0.000595	1.39316E-09	7.17794E-06	-0.00029844	-28.7951	-0.09512
2.03	8.903	0.000303	0.000615	1.25026E-09	7.99834E-06	-0.00031984	-30.8595	-0.10194
2.1	8.944	0.000302	0.000634	1.13763E-09	8.79023E-06	-0.00034112	-32.9127	-0.10872
2.17	8.984	0.000301	0.000654	1.03753E-09	9.63829E-06	-0.00036237	-34.963	-0.1155
2.24	9.022	0.000301	0.000674	9.50605E-10	1.05196E-05	-0.00038357	-37.0083	-0.12225
2.31	9.052	0.0003	0.000693	8.87156E-10	1.1272E-05	-0.00040455	-39.0328	-0.12894
2.38	9.086	0.0003	0.000713	8.20352E-10	1.21899E-05	-0.00042561	-41.0652	-0.13565
2.45	9.115	0.000299	0.000732	7.67361E-10	1.30317E-05	-0.00044652	-43.082	-0.14232
2.52	9.142	0.000298	0.000752	7.21107E-10	1.38676E-05	-0.00046733	-45.0902	-0.14895
2.59	9.167	0.000298	0.000771	6.80769E-10	1.46893E-05	-0.00048805	-47.089	-0.15555
2.66	9.184	0.000297	0.00079	6.54636E-10	1.52757E-05	-0.00050844	-49.0571	-0.16205
2.73	9.211	0.000296	0.000809	6.15177E-10	1.62555E-05	-0.00052915	-51.0553	-0.16866
2.8	9.228	0.000296	0.000828	5.91562E-10	1.69044E-05	-0.00054945	-53.0136	-0.17512
2.87	9.252	0.000295	0.000847	5.59758E-10	1.78649E-05	-0.00056998	-54.9942	-0.18167
2.94	9.272	0.000295	0.000866	5.34564E-10	1.87068E-05	-0.0005903	-56.9555	-0.18815
3.01	9.289	0.000294	0.000885	5.14044E-10	1.94536E-05	-0.00061046	-58.8999	-0.19457
3.08	9.306	0.000293	0.000904	4.94311E-10	2.02302E-05	-0.00063056	-60.8395	-0.20098
3.15	9.321	0.000293	0.000922	4.77529E-10	2.09411E-05	-0.00065052	-62.7651	-0.20734
3.22	9.338	0.000292	0.000941	4.59198E-10	2.17771E-05	-0.00067052	-64.6952	-0.21371
3.29	9.353	0.000292	0.000959	4.43609E-10	2.25424E-05	-0.00069038	-66.6109	-0.22004
3.36	9.368	0.000291	0.000978	4.28549E-10	2.33346E-05	-0.00071018	-68.5217	-0.22635
3.43	9.383	0.00029	0.000996	4.14E-10	2.41546E-05	-0.00072993	-70.4278	-0.23265
3.5	9.395	0.00029	0.001014	4.02717E-10	2.48313E-05	-0.00074947	-72.3126	-0.23888

0.010 M NaNO$_3$

Vol.of NaOH	pH	C_A	C_B	[H$^+$]	[OH$^-$]	[(C_A- C_B-[H$^+$]-[OH$^-$])]	[(C_A- C_B-[H$^+$]-[OH$^-$])] x96485	[(C_A- C_B-[H$^+$]-[OH$^-$])] x96485/302.72 surface charge density (6_0)
0	3.724	0.000323	0	0.000189	5.29663E-11	0.000133781	12.9079	0.04264
0.07	3.815	0.000322	2.25E-05	0.000153	6.53131E-11	0.000146215	14.10758	0.046603
0.14	3.923	0.000321	4.5E-05	0.000119	8.37529E-11	0.000156773	15.12627	0.049968
0.21	4.048	0.00032	6.73E-05	8.95E-05	1.11686E-10	0.000163587	15.78373	0.05214
0.28	4.199	0.00032	8.95E-05	6.32E-05	1.58125E-10	0.000166938	16.10698	0.053208
0.35	4.376	0.000319	0.000112	4.21E-05	2.37684E-10	0.000165264	15.94546	0.052674
0.42	4.586	0.000318	0.000134	2.59E-05	3.85478E-10	0.000158654	15.30769	0.050567
0.49	4.816	0.000318	0.000156	1.53E-05	6.54636E-10	0.00014668	14.15241	0.046751
0.56	5.075	0.000317	0.000177	8.41E-06	1.1885E-09	0.000131002	12.63971	0.041754
0.63	5.347	0.000316	0.000199	4.5E-06	2.22331E-09	0.000112478	10.85239	0.03585
0.7	5.627	0.000315	0.000221	2.36E-06	4.23643E-09	9.22725E-05	8.902913	0.02941
0.77	5.899	0.000315	0.000242	1.26E-06	7.92501E-09	7.11256E-05	6.862552	0.02267
0.84	6.158	0.000314	0.000264	6.95E-07	1.4388E-08	4.95418E-05	4.780045	0.01579
0.91	6.396	0.000313	0.000285	4.02E-07	2.48886E-08	2.77776E-05	2.680126	0.008853
0.98	6.609	0.000313	0.000306	2.46E-07	4.06443E-08	5.96723E-06	0.575748	0.001902
1.05	6.811	0.000312	0.000328	1.55E-07	6.47143E-08	-1.582E-05	-1.52638	-0.00504
1.12	7.012	0.000311	0.000349	9.73E-08	1.02802E-07	-3.756E-05	-3.62397	-0.01197
1.19	7.203	0.000311	0.00037	6.27E-08	1.59588E-07	-5.9247E-05	-5.71643	-0.01888
1.26	7.397	0.00031	0.000391	4.01E-08	2.49459E-07	-8.0885E-05	-7.80416	-0.02578
1.33	7.581	0.000309	0.000411	2.62E-08	3.81066E-07	-0.00010248	-9.88775	-0.03266
1.4	7.735	0.000309	0.000432	1.84E-08	5.4325E-07	-0.00012402	-11.9659	-0.03953
1.47	7.852	0.000308	0.000453	1.41E-08	7.11214E-07	-0.00014547	-14.0361	-0.04637
1.54	7.962	0.000307	0.000473	1.09E-08	9.1622E-07	-0.00016688	-16.1011	-0.05319
1.61	8.039	0.000307	0.000494	9.14E-09	1.09396E-06	-0.00018816	-18.1548	-0.05997
1.68	8.112	0.000306	0.000514	7.73E-09	1.2942E-06	-0.00020938	-20.2021	-0.06674
1.75	8.176	0.000305	0.000534	6.67E-09	1.49968E-06	-0.00023051	-22.2411	-0.07347

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (δ_0)
1.82	8.225	0.000305	0.000555	5.96E-09	1.6788E-06	-0.00025153	-24.2691	-0.08017
1.89	8.274	0.000304	0.000575	5.32E-09	1.87932E-06	-0.00027248	-26.2906	-0.08685
1.96	8.305	0.000303	0.000595	4.95E-09	2.01837E-06	-0.00029329	-28.2976	-0.09348
2.03	8.33	0.000303	0.000615	4.68E-09	2.13796E-06	-0.00031398	-30.2944	-0.10007
2.1	8.345	0.000302	0.000634	4.52E-09	2.21309E-06	-0.00033454	-32.2785	-0.10663
2.17	8.361	0.000301	0.000654	4.36E-09	2.29615E-06	-0.00035503	-34.255	-0.11316
2.24	8.383	0.000301	0.000674	4.14E-09	2.41546E-06	-0.00037546	-36.2267	-0.11967
2.31	8.406	0.0003	0.000693	3.93E-09	2.54683E-06	-0.00039583	-38.1913	-0.12616
2.38	8.459	0.0003	0.000713	3.48E-09	2.8774E-06	-0.0004163	-40.1669	-0.13269
2.45	8.521	0.000299	0.000732	3.01E-09	3.31894E-06	-0.0004368	-42.1451	-0.13922
2.52	8.582	0.000298	0.000752	2.62E-09	3.81944E-06	-0.00045728	-44.1209	-0.14575
2.59	8.638	0.000298	0.000771	2.3E-09	4.3451E-06	-0.0004777	-46.0911	-0.15226
2.66	8.695	0.000297	0.00079	2.02E-09	4.9545E-06	-0.00049812	-48.0614	-0.15877
2.73	8.753	0.000296	0.000809	1.77E-09	5.66239E-06	-0.00051856	-50.0333	-0.16528
2.8	8.809	0.000296	0.000828	1.55E-09	6.44169E-06	-0.00053899	-52.0042	-0.17179
2.87	8.858	0.000295	0.000847	1.39E-09	7.21107E-06	-0.00055932	-53.9663	-0.17827
2.94	8.905	0.000295	0.000866	1.24E-09	8.03526E-06	-0.00057963	-55.9259	-0.18474
3.01	8.94	0.000294	0.000885	1.15E-09	8.70964E-06	-0.00059971	-57.8634	-0.19114
3.08	8.974	0.000293	0.000904	1.06E-09	9.4189E-06	-0.00061975	-59.7964	-0.19753
3.15	8.996	0.000293	0.000922	1.01E-09	9.90832E-06	-0.00063948	-61.7007	-0.20382
3.22	9.01	0.000292	0.000941	9.77E-10	1.02329E-05	-0.00065898	-63.5814	-0.21003
3.29	9.023	0.000292	0.000959	9.48E-10	1.05439E-05	-0.00067838	-65.4533	-0.21622
3.36	9.035	0.000291	0.000978	9.23E-10	1.08393E-05	-0.00069769	-67.3162	-0.22237
3.43	9.047	0.00029	0.000996	8.97E-10	1.11429E-05	-0.00071692	-69.1724	-0.2285
3.5	9.059	0.00029	0.001014	8.73E-10	1.14551E-05	-0.00073609	-71.022	-0.23461

0.005 M NaNO₃

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A - C_B - [H^+]-[OH^-])]$	$[(C_A - C_B - [H^+]-[OH^-])]$ x96485	$[(C_A - C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (δ_0)
0	3.687	0.000323	0	0.000206	4.86407E-11	0.000116992	11.28792844	0.037288347
0.07	3.761	0.000322	2.25E-05	0.000173	5.76766E-11	0.000125944	12.15167301	0.040141626
0.14	3.852	0.000321	4.5E-05	0.000141	7.11214E-11	0.000135567	13.08021117	0.043208943
0.21	3.962	0.00032	6.73E-05	0.000109	9.1622E-11	0.00014398	13.89189809	0.045890255
0.28	4.092	0.00032	8.95E-05	8.09E-05	1.23595E-10	0.000149269	14.40224982	0.047576142
0.35	4.245	0.000319	0.000112	5.69E-05	1.75792E-10	0.000150451	14.51626997	0.047952795
0.42	4.429	0.000318	0.000134	3.72E-05	2.68534E-10	0.000147356	14.21767837	0.046966432
0.49	4.644	0.000318	0.000156	2.27E-05	4.40555E-10	0.000139257	13.43622009	0.044384977
0.56	4.894	0.000317	0.000177	1.28E-05	7.8343E-10	0.000126652	12.22000008	0.040367336
0.63	5.174	0.000316	0.000199	6.7E-06	1.49279E-09	0.000110277	10.640097	0.035148312
0.7	5.48	0.000315	0.000221	3.31E-06	3.01995E-09	9.13229E-05	8.811289313	0.02910706
0.77	5.805	0.000315	0.000242	1.57E-06	6.38263E-09	7.08222E-05	6.833280721	0.022572941
0.84	6.126	0.000314	0.000264	7.48E-07	1.3366E-08	4.94897E-05	4.775015714	0.015773704
0.91	6.422	0.000313	0.000285	3.78E-07	2.64241E-08	2.77995E-05	2.682230704	0.008860434
0.98	6.697	0.000313	0.000306	2.01E-07	4.97737E-08	6.00323E-06	0.579221232	0.001913389
1.05	6.942	0.000312	0.000328	1.14E-07	8.74984E-08	-1.5802E-05	-1.52469555	-0.005036653
1.12	7.198	0.000311	0.000349	6.34E-08	1.57761E-07	-3.7581E-05	-3.62600746	-0.01197809
1.19	7.441	0.000311	0.00037	3.62E-08	2.76058E-07	-5.9337E-05	-5.72511345	-0.018912241
1.26	7.7	0.00031	0.000391	2E-08	5.01187E-07	-8.1116E-05	-7.82650661	-0.025853946
1.33	7.953	0.000309	0.000411	1.11E-08	8.97429E-07	-0.00010298	-9.93611699	-0.032822797
1.4	8.192	0.000309	0.000432	6.43E-09	1.55597E-06	-0.00012502	-12.0624758	-0.039846974
1.47	8.405	0.000308	0.000453	3.94E-09	2.54097E-06	-0.00014729	-14.2116526	-0.046946527
1.54	8.57	0.000307	0.000473	2.69E-09	3.71535E-06	-0.00016967	-16.3703827	-0.054077638
1.61	8.706	0.000307	0.000494	1.97E-09	5.08159E-06	-0.00019214	-18.5388929	-0.061241057
1.68	8.819	0.000306	0.000514	1.52E-09	6.59174E-06	-0.00021467	-20.7125885	-0.068421606
1.75	8.917	0.000305	0.000534	1.21E-09	8.26038E-06	-0.00023727	-22.892921	-0.075624079

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (δ_0)
1.82	8.998	0.000305	0.000555	1E-09	9.95405E-06	-0.0002598	-25.0670647	-0.082806107
1.89	9.06	0.000304	0.000575	8.71E-10	1.14815E-05	-0.00028208	-27.2166213	-0.089906915
1.96	9.125	0.000303	0.000595	7.5E-10	1.33352E-05	-0.0003046	-29.3891477	-0.097083601
2.03	9.175	0.000303	0.000615	6.68E-10	1.49624E-05	-0.0003268	-31.5313702	-0.104160182
2.1	9.226	0.000302	0.000634	5.94E-10	1.68267E-05	-0.00034915	-33.6880869	-0.111284642
2.17	9.268	0.000301	0.000654	5.4E-10	1.85353E-05	-0.00037126	-35.8214287	-0.118331887
2.24	9.309	0.000301	0.000674	4.91E-10	2.03704E-05	-0.00039342	-37.9586884	-0.125392073
2.31	9.343	0.0003	0.000693	4.54E-10	2.20293E-05	-0.00041531	-40.070704	-0.132368869
2.38	9.378	0.0003	0.000713	4.19E-10	2.38781E-05	-0.0004373	-42.1928656	-0.139379181
2.45	9.409	0.000299	0.000732	3.9E-10	2.56448E-05	-0.00045913	-44.298969	-0.146336446
2.52	9.437	0.000298	0.000752	3.66E-10	2.73527E-05	-0.00048081	-46.3913073	-0.15324824
2.59	9.463	0.000298	0.000771	3.44E-10	2.90402E-05	-0.0005024	-48.4736526	-0.160127024
2.66	9.492	0.000297	0.00079	3.22E-10	3.10456E-05	-0.00052421	-50.5786799	-0.167080734
2.73	9.512	0.000296	0.000809	3.08E-10	3.25087E-05	-0.00054541	-52.6234563	-0.173835413
2.8	9.532	0.000296	0.000828	2.94E-10	3.40408E-05	-0.00056659	-54.6670011	-0.180586024
2.87	9.554	0.000295	0.000847	2.79E-10	3.58096E-05	-0.00058792	-56.7255515	-0.187386203
2.94	9.573	0.000295	0.000866	2.67E-10	3.74111E-05	-0.00060901	-58.7601621	-0.194107301
3.01	9.596	0.000294	0.000885	2.54E-10	3.94457E-05	-0.00063045	-60.8288361	-0.200940923
3.08	9.615	0.000293	0.000904	2.43E-10	4.12098E-05	-0.00065154	-62.863705	-0.207662873
3.15	9.63	0.000293	0.000922	2.34E-10	4.2658E-05	-0.00067223	-64.8604578	-0.214258912
3.22	9.647	0.000292	0.000941	2.25E-10	4.43609E-05	-0.0006931	-66.8741891	-0.220911037
3.29	9.666	0.000292	0.000959	2.16E-10	4.63447E-05	-0.00071418	-68.9074735	-0.227627753
3.36	9.679	0.000291	0.000978	2.09E-10	4.77529E-05	-0.0007346	-70.8777175	-0.234136223
3.43	9.694	0.00029	0.000996	2.02E-10	4.94311E-05	-0.00075521	-72.8665443	-0.240706079
3.5	9.708	0.00029	0.001014	1.96E-10	5.10505E-05	-0.00077569	-74.8422931	-0.247232733

0.001 M NaNO₃

Vol.of NaOH	pH	C_A	C_B	[H⁺]	[OH⁻]	[(C_A- C_B- [H⁺]-[OH⁻])]	[(C_A- C_B- [H⁺]-[OH⁻])] x96485	[(C_A- C_B-[H⁺]- [OH⁻])] x96485/302.72 surface charge density (δ₀)
0	3.717	0.000323	0	0.000192	5.21195E-11	0.000130714	12.61191	0.04166198
0.07	3.8	0.000322	2.25E-05	0.000158	6.30957E-11	0.000140835	13.58844	0.04488781
0.14	3.905	0.000321	4.5E-05	0.000124	8.03526E-11	0.000151721	14.63876	0.04835743
0.21	4.011	0.00032	6.73E-05	9.75E-05	1.02565E-10	0.000155625	15.01547	0.04960185
0.28	4.155	0.00032	8.95E-05	7E-05	1.42889E-10	0.000160195	15.45638	0.05105835
0.35	4.314	0.000319	0.000112	4.85E-05	2.06063E-10	0.000158807	15.32254	0.05061621
0.42	4.498	0.000318	0.000134	3.18E-05	3.14775E-10	0.000152827	14.74549	0.04870999
0.49	4.726	0.000318	0.000156	1.88E-05	5.32108E-10	0.000143162	13.81303	0.04562973
0.56	4.977	0.000317	0.000177	1.05E-05	9.48418E-10	0.000128872	12.43423	0.04107502
0.63	5.255	0.000316	0.000199	5.56E-06	1.79887E-09	0.000111417	10.75004	0.0355115
0.7	5.543	0.000315	0.000221	2.86E-06	3.4914E-09	9.17696E-05	8.854385	0.02924942
0.77	5.845	0.000315	0.000242	1.43E-06	6.99842E-09	7.09594E-05	6.846522	0.02261668
0.84	6.138	0.000314	0.000264	7.28E-07	1.37404E-08	4.95097E-05	4.776947	0.01578008
0.91	6.408	0.000313	0.000285	3.91E-07	2.55859E-08	2.77879E-05	2.681115	0.00885675
0.98	6.658	0.000313	0.000306	2.2E-07	4.54988E-08	5.98862E-06	0.577812	0.00190874
1.05	6.885	0.000312	0.000328	1.3E-07	7.67361E-08	-1.5808E-05	-1.5252	-0.0050383
1.12	7.105	0.000311	0.000349	7.85E-08	1.2735E-07	-3.7566E-05	-3.62453	-0.0119732
1.19	7.294	0.000311	0.00037	5.08E-08	1.96789E-07	-5.9272E-05	-5.71887	-0.0188916
1.26	7.487	0.00031	0.000391	3.26E-08	3.06902E-07	-8.0935E-05	-7.80898	-0.025796
1.33	7.666	0.000309	0.000411	2.16E-08	4.63447E-07	-0.00010256	-9.89525	-0.0326878
1.4	7.838	0.000309	0.000432	1.45E-08	6.88652E-07	-0.00012416	-11.9796	-0.0395731
1.47	8.012	0.000308	0.000453	9.73E-09	1.02802E-06	-0.00014579	-14.0662	-0.0464662
1.54	8.171	0.000307	0.000473	6.75E-09	1.48252E-06	-0.00016744	-16.1553	-0.0533673
1.61	8.32	0.000307	0.000494	4.79E-09	2.0893E-06	-0.00018915	-18.2505	-0.0602882
1.68	8.444	0.000306	0.000514	3.6E-09	2.77971E-06	-0.00021086	-20.345	-0.0672073
1.75	8.555	0.000305	0.000534	2.79E-09	3.58922E-06	-0.0002326	-22.4424	-0.0741358

Vol.of NaOH	pH	C_A	C_B	$[H^+]$	$[OH^-]$	$[(C_A- C_B-[H^+]-[OH^-])]$	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485	$[(C_A- C_B-[H^+]-[OH^-])]$ x96485/302.72 surface charge density (δ_0)
1.82	8.655	0.000305	0.000555	2.21E-09	4.51856E-06	-0.00025437	-24.5427	-0.0810741
1.89	8.734	0.000304	0.000575	1.85E-09	5.42001E-06	-0.00027602	-26.6319	-0.0879753
1.96	8.805	0.000303	0.000595	1.57E-09	6.38263E-06	-0.00029765	-28.7184	-0.0948679
2.03	8.861	0.000303	0.000615	1.38E-09	7.26106E-06	-0.0003191	-30.7884	-0.1017058
2.1	8.917	0.000302	0.000634	1.21E-09	8.26038E-06	-0.00034059	-32.8616	-0.1085545
2.17	8.961	0.000301	0.000654	1.09E-09	9.14113E-06	-0.00036187	-34.9151	-0.1153379
2.24	9	0.000301	0.000674	1E-09	0.00001	-0.00038305	-36.9581	-0.1220869
2.31	9.04	0.0003	0.000693	9.12E-10	1.09648E-05	-0.00040424	-39.0032	-0.1288425
2.38	9.071	0.0003	0.000713	8.49E-10	1.17761E-05	-0.0004252	-41.0252	-0.1355221
2.45	9.103	0.000299	0.000732	7.89E-10	1.26765E-05	-0.00044616	-43.0478	-0.1422032
2.52	9.128	0.000298	0.000752	7.45E-10	1.34276E-05	-0.00046689	-45.0478	-0.1488101
2.59	9.157	0.000298	0.000771	6.97E-10	1.43549E-05	-0.00048771	-47.0568	-0.1554465
2.66	9.179	0.000297	0.00079	6.62E-10	1.51008E-05	-0.00050827	-49.0403	-0.1619988
2.73	9.204	0.000296	0.000809	6.25E-10	1.59956E-05	-0.00052889	-51.0302	-0.1685723
2.8	9.226	0.000296	0.000828	5.94E-10	1.68267E-05	-0.00054937	-53.0061	-0.1750995
2.87	9.246	0.000295	0.000847	5.68E-10	1.76198E-05	-0.00056973	-54.9705	-0.1815887
2.94	9.268	0.000295	0.000866	5.4E-10	1.85353E-05	-0.00059013	-56.939	-0.1880912
3.01	9.287	0.000294	0.000885	5.16E-10	1.93642E-05	-0.00061037	-58.8913	-0.1945405
3.08	9.316	0.000293	0.000904	4.83E-10	2.07014E-05	-0.00063103	-60.885	-0.2011264
3.15	9.314	0.000293	0.000922	4.85E-10	2.06063E-05	-0.00065018	-62.7328	-0.2072305
3.22	9.331	0.000292	0.000941	4.67E-10	2.14289E-05	-0.00067017	-64.6616	-0.2136021
3.29	9.351	0.000292	0.000959	4.46E-10	2.24388E-05	-0.00069027	-66.6009	-0.2200084
3.36	9.37	0.000291	0.000978	4.27E-10	2.34423E-05	-0.00071029	-68.5321	-0.2263878
3.43	9.38	0.00029	0.000996	4.17E-10	2.39883E-05	-0.00072977	-70.4117	-0.2325969
3.5	9.392	0.00029	0.001014	4.06E-10	2.46604E-05	-0.0007493	-72.2961	-0.2388216

APPENDIX G

## Determination of the capacitance(C)

The capacitance(C) can be obtained from the slope of the plot of the PZC-pH values

against surface charge density,σ_0,of goethite using equation (48),i.e.,

$$PZC - PH = \log e.\left(\frac{F}{RT} \frac{\sigma_0}{C} \right)$$. Linear regression of the data was carried out for each

system. The linear relationship and the capacitance(C) was obtained as follow:

0.500 M NaNO₃ System

7.0(PZC)-pH	16.75X surface charge
2.392	1.486124362
2.188	1.402448672
1.963	1.303345905
1.733	1.191756731
1.508	1.072312732
1.293	0.948534511
1.089	0.82258852
0.893	0.695704335
0.709	0.568484729
0.533	0.441328372
0.367	0.314425732
0.205	0.187902298
0.046	0.061808192
-0.108	-0.063835059
-0.262	-0.189029141
-0.411	-0.313785862
-0.559	-0.43814576
-0.708	-0.562178968
-0.845	-0.685873221

$y = 0.804x + 0.02$

$R^2 = 0.9983$
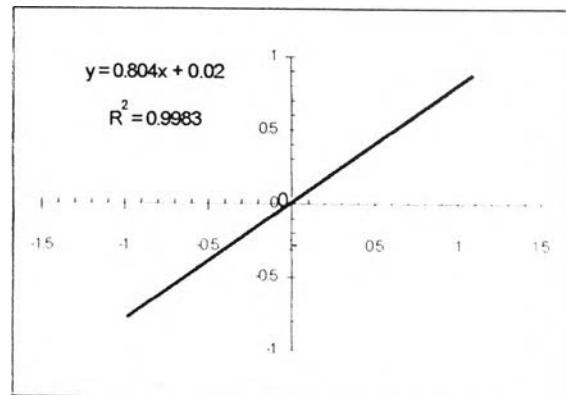
Slope= C= 0.80±0.02

0.100 M NaNO₃ System

7.0(PZC)-pH	16.75X surface charge
2.901	1.297108997
2.733	1.309302024
2.517	1.298828446
2.269	1.25216179
2.005	1.174840845
1.733	1.07802336
1.471	0.969687093
1.227	0.855595807
1.001	0.738897743
0.784	0.621170735
0.58	0.503067269
0.38	0.384992001
0.193	0.267100219
0.003	0.149505967
-0.181	0.032225772
-0.36	-0.084742726
-0.543	-0.201469229
-0.715	-0.317985465
-0.879	-0.434382428
-1.036	-0.550780487
-1.178	-0.667174422

$y = 0.6401x + 0.1147$

$R^2 = 0.9957$
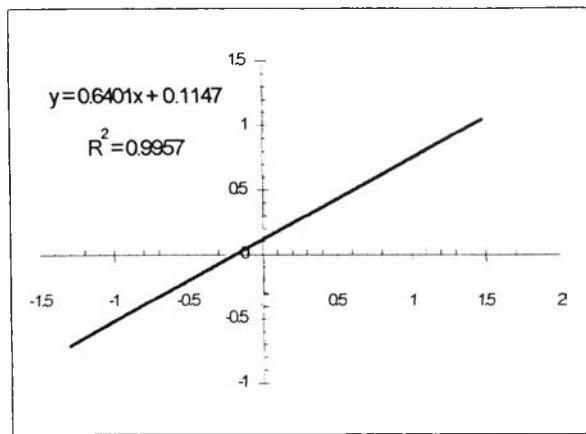
Slope= C= 0.64±0.11

0.010 M NaNO₃ System

7.0(PZC)-pH	16.75X surface charge
3.306	0.714215745
3.215	0.780595968
3.107	0.836961361
2.982	0.873340048
2.831	0.891226075
2.654	0.8822888
2.444	0.847000142
2.214	0.783076135
1.955	0.699376291
1.683	0.600481003
1.403	0.492612955
1.131	0.379716416
0.872	0.264487813
0.634	0.148295825
0.421	0.03185709
0.219	-0.084457114
0.018	-0.200520515
-0.173	-0.316299373
-0.367	-0.431817196
-0.551	-0.547105759
-0.705	-0.662094211
-0.822	-0.776639891
-0.932	-0.890900685
-1.009	-1.004537303
-1.082	-1.117813186
-1.146	-1.230639298

$y = 0.5447x - 0.23$

$R^2 = 0.9953$
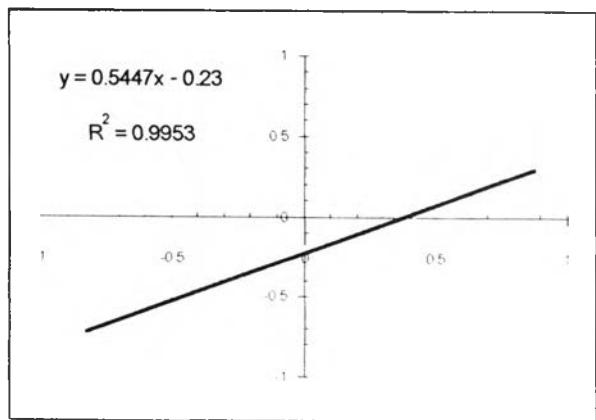
Slope= C= 0.54±0.23

0.005 M NaNO₃ System

7.0(PZC)-pH	16.75X surface charge
3.313	0.624579814
3.239	0.672372235
3.148	0.723749792
3.038	0.768661777
2.908	0.796900385
2.755	0.803209309
2.571	0.78668774
2.356	0.743448356
2.106	0.676152885
1.826	0.588734225
1.52	0.487543261
1.195	0.378096763
0.874	0.264209544
0.578	0.148412276
0.303	0.032049272
0.058	-0.084363935
-0.198	-0.200633011
-0.441	-0.316780029
-0.7	-0.4330536
-0.953	-0.549781843
-1.192	-0.667436807

$y = 0.4537x - 0.1218$

$R^2 = 0.9982$
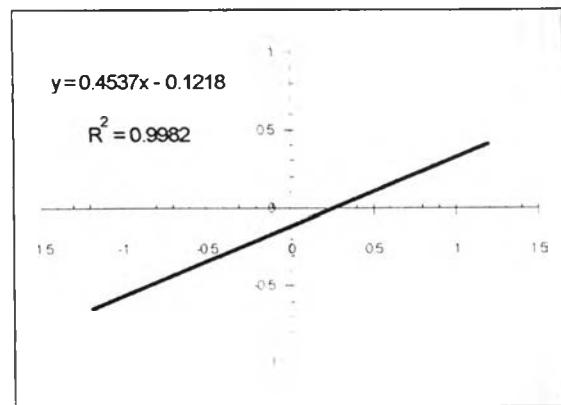
Slope= C= 0.45±0.12

0.001 M NaNO₃ System

7.0(PZC)-pH	16.75X surface charge
3.283	0.697838087
3.2	0.751870848
3.095	0.809986918
2.989	0.830830964
2.845	0.855227392
2.686	0.847821482
2.502	0.815892341
2.274	0.764297959
2.023	0.688006635
1.745	0.594817632
1.457	0.489927843
1.155	0.37882945
0.862	0.264316399
0.592	0.148350561
0.342	0.031971318
0.115	-0.084392052
-0.105	-0.200551467
-0.294	-0.316434737
-0.487	-0.432083808
-0.666	-0.547520662
-0.838	-0.662849715
-1.012	-0.778308065
-1.171	-0.893901706

$y = 0.5048x - 0.1775$

$R^2 = 0.9923$
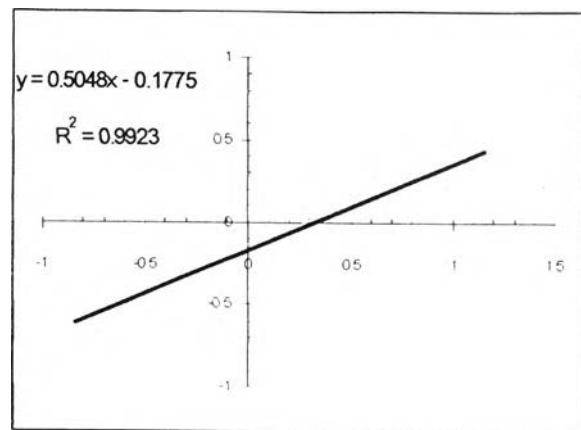
Slope= C= 0.50±0.18

VITA

Miss Kanokwan Janhan was born on December 27, 1976 in Mahasarakham, Thailand. She received the Bachelor Degree of Science in Chemistry from Khon Kaen University in 1998. Since then, she has been a graduate student stydying in the field of Physical Chemistry at Chulalongkorn University. She graduated with a Master Degree of Science in Chemistry in the second semester 2001.