



ANALYSIS OF THE VISIBLE SPECTRA
OF CONCENTRATED CHROMIC CHLORIDE
SOLUTIONS

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INTRODUCTION

In the development of the NASA Redox Energy Storage System, the electrical storage efficiency has been low due to the complex chemical reaction of the chromium II and III species. This paper describes several studies dealing with the processes occurring at the catalyzed carbon electrode during the charging and discharging of the system.

The Redox Energy Storage System is an electrochemical device that employs the oxidation and reduction of two soluble redox couples for charging and discharging. In a Redox flow cell there are two active electrolyte solutions separated by a highly selective ion exchange membrane (fig. 1) (1). Each electrode consists of porous carbon felt, a few millimeters in width. On the chromium side, the carbon felt is catalyzed by trace amounts of gold and lead because the rate of reduction of Cr(III) to Cr(II) is slow on most surfaces (4,5, and 7). This catalyst also improves the cell discharge rate. On the iron side no catalyst is needed (1).

In the aqueous chromic chloride, the complex ions, $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ and $\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2^+$, exist in equilibrium with $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ (3). Depending on whether the cell is being charged or discharged, there are distinctive differences observed at the same state of charge in the chromium solutions (9). In fig. 2 the complete charge cycle is observed

using open-circuit voltage behavior. Above 50 percent state-of-charge, the charging rate decreases considerably.

$\text{Cr}(\text{H}_2\text{O})_6^{+3}$ and $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ have been identified as the predominant Cr(III) species present in the acidified CrCl_3 solutions of the NASA Redox System and are shown in figure 3 (1,6 and 8). The reactions occurring at the catalyzed carbon felt electrode during charge-discharge cycles have been followed spectrophotometrically and potentiometrically (1). Figure 4 is a typical spectrum and figure 5 shows the emf data plotted versus the ratios of Cr(II) to Cr(III) calculated from the spectra using Beer's Law.

The concentration of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ is found to decrease much more rapidly with the increasing state-of-charge than does the concentration of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$, indicating that $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ is predominantly reduced during the charging cycle (1). There is a rapid rise in $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ concentration, and a slow rise in the concentration of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$, as discharge takes place. Electrode potential data also indicates that $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ is the primary electroactive species. This can be explained as the reduction of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ via an inner-sphere chloride-bridged electrode reaction and the oxidation of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^+$ via an inner-sphere chloride-bridged electrode reaction shown in fig. 7 (1). There is also a slowly attained equilibrium between $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ and $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$.

The spectra was analyzed using a DuPont 310 curve resolver and the visible spectra of the complex ions present in the solution which are shown in figure 6 (1).

The Frank-Condon principle, which states that the motions of heavy atoms are negligibly slow with respect to the rapid motions of electrons dictates that the atomic geometry of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ during reduction should remain the same as well as the $\text{Cr}(\text{II})$ species during oxidation (4). The reaction pathway determined at a dropping mercury electrode and a catalyzed carbon electrode found the complexes $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ and $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ to be involved in the oxidation and reduction reactions (1). The electrode potential data shows that $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ and Cr^{+2} obey the Nernst equation in the discharge mode and in the charge mode. $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ and $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^+$ appear to be the electro-active species. This activity can be explained by the unique atomic structure (octahedral) as well as the high activity of the chloride ion. The chloride ion forms a bridged inner-sphere pathway which is much more active than the H_2O pathway on the $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ (7). The ligands in the reactant's primary coordination sphere penetrate the layer of solvent molecules and ions specifically coordinated to the electrode surface. Thus, the crystal field that stabilized the octahedral $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ is overcome. Reduction can now occur in the charge mode because the energy of activation is lowered.

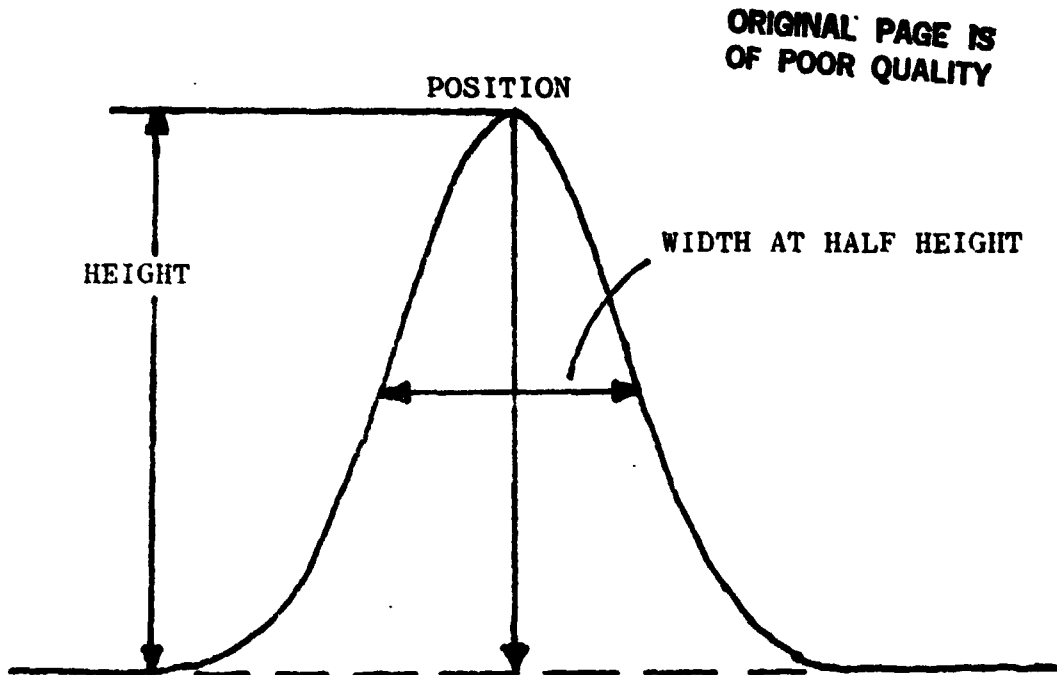
The goal of this research was to analyze the visible spectra of acidified chromic chloride solutions using curve resolving techniques previously developed, to develop new computer techniques to analyze the spectra, and compare the results of the two methods. This comparison will be helpful in assessing the validity of using curve resolving techniques in previous studies and in carrying out future studies on the temperature dependence of chromium (III) complex concentrations.

EXPERIMENTAL PROCEDURES AND CALCULATIONS

Solutions of 1M CrCl_3 in 1N HCl and 1M CrCl_3 in 2N HCl were placed in 25°C, 40°C, 55°C, and 69.5°C water baths and the spectra recorded after 2, 4, 6, and 24 hours to detect any equilibrium changes in solution (3). Two samples were used, one 10ml and the other 25ml.

Analysis of the spectral data (figures 8-14) were first curved out with the Dupont 310 curve resolver. To resolve overlapping peaks, the instrument generates a series of component peaks and synthesizes a sum curve matching the original data. The resolver generates, on each of its function channels, peak shapes corresponding to many distributions. Since the visible spectrophotometer gives Gaussian curve functions, the 310's individual peak parameters of height, width, and horizontal position are independently varied to fit this distribution. The data obtained from the spectrophotometer are displayed in some

type of X-Y readout with the peak overlap occurring on the X-axis. For example, the Gaussian function is illustrated in the figure below with important parameters shown:



TYPICAL DISTRIBUTION FUNCTION

The analog computer in the 310 adds the individual distribution functions together algebraically, and compares the resulting envelope with the actual experimental data. When resolving overlapping curve envelopes into their individual component curves, the 310 comes to within 1 percent (DuPont 310 Curve Resolver Manual, 1968).

The experimenter fits each curve to his satisfaction by varying each parameter independently. This can be

achieved by viewing each component on the screen individually and making appropriate adjustments. When every component is combined on the screen, the readout should fit the total curve envelope.

When resolving each curve, data previously obtained from the spectra of the individual components was used. The maxima of the absorption of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ are 605 and 430, and $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ are 575 and 407. The molar absorptivity ratios of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ and the $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ are 0.824 liter $\text{mol}^{-1}\text{cm}^{-1}$ and 0.863 liter $\text{mol}^{-1}\text{cm}^{-1}$ respectively. Thus, the peaks were positioned and the heights determined according to the ratio of the molar absorptivities. Figures 8-14 show the spectra resolved into the $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ and $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ peaks.

The calculation of the concentrations of the complexes utilize Beer's Law:

$$A = abc \text{ or } c = A/ab$$

A = absorbance

a = molar absorptivity (liter $\text{mol}^{-1}\text{cm}^{-1}$)

b = width of sample cell (cm)

c = concentration of sample (mol liter $^{-1}$)

The molar absorptivities of the individual species were calculated at arbitrary wavelengths from the spectra of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ and $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$. The complex ions were prepared according to a procedure by Angelici and chromium

concentrations determined by alkaline peroxide oxidation to chromate (9).

A computer program was developed to calculate the concentrations of the chromium (III) complexes from calculated molar absorptivities and is given in table 1. Absorbance values were obtained from the acidified chromium (III) solutions spectra. Using Beer's Law each set of data is compared against the other, giving a total of 45 possible combinations. These simultaneous equations are used to solve for the concentrations:

$$A_1 = a_{1H}b_1c_H + a_{1P}b_1c_P$$

$$A_2 = a_{2H}b_2c_H + a_{2P}b_2c_P$$

A_1 = absorbance at first wavelength

A_2 = absorbance at second wavelength

a_{1H} = molar absorptivity at first wavelength of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$

a_{1P} = molar absorptivity at first wavelength of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$

a_{2P} = molar absorptivity at second wavelength of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$

a_{2H} = molar absorptivity at second wavelength of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$

$b_1 = b_2$ = cell width used

c_H = concentration of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$

c_P = concentration of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$

To avoid extremely erroneous values, a retaining sub-program was added. After the 45 concentration values are averaged, the sub-program is activated. Values greater than the average by an arbitrarily chosen retaining percentage are expelled. The final concentration value is then cal-

culated from this new set of data.

To ensure the reliability of each of these methods, their concentrations must be compared. Since the peaks of the spectra relay the most accurate data, we chose these as our data points. For example, from spectra #82 we can calculate the concentration of each species as follows:

PENTA COMPLEX:

First Peak -

$$a = 17.8 \text{ liter mol}^{-1} \text{cm}^{-1}$$

$$A = 0.897$$

$$b = 0.1 \text{cm}$$

$$c = A/ab = 0.897 / (17.8 \text{ liter/mol}^{-1} \text{cm}^{-1})(0.1 \text{cm})$$

$$= 0.5039 \text{ mol/liter}$$

Second Peak -

$$a = 21.6 \text{ liter mol}^{-1} \text{cm}^{-1}$$

$$A = 1.040$$

$$b = 0.1 \text{cm}$$

$$c = A/ab = 1.040 / (21.6 \text{ liter/mol}^{-1} \text{cm}^{-1})(0.1 \text{cm})$$

$$= 0.4815 \text{ mol/liter}$$

$$\text{average} = 0.4927 \text{ mol/liter}$$

$$\text{Computed value for concentration of } \text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2} = 0.6207 \text{ mol/liter}$$

$$\text{Percent difference} = 0.6207 - 0.4927 / 0.4927 \times 100 = 25.9 \text{ percent}$$

HEXA COMPLEX:

First Peak -

$$a = 13.9 \text{ liter mol}^{-1} \text{cm}^{-1}$$

$$A = 0.597$$

$$b = 0.1 \text{cm}$$

$$c = A/ab = 0.597 / (13.9 \text{ liter mol}^{-1} \text{cm}^{-1})(0.1 \text{cm})$$

$$= 0.4295 \text{ mol/liter}$$

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Second Peak -

$$a = 16.1 \text{ liter mol}^{-1} \text{cm}^{-1}$$

$$A = 0.706$$

$$b = 0.1 \text{cm}$$

$$c = A/ab = 0.706 / (16.1 \text{ liter mol}^{-1} \text{cm}^{-1})(0.1 \text{cm}) \\ = 0.4385 \text{ mol/liter}$$

$$\text{Average} = 0.4340 \text{ mol/liter}$$

$$\text{Computed value for concentration of } \text{Cr}(\text{H}_2\text{O})_6^{+3} = 0.3363 \\ \text{mol/liter}$$

$$\text{Percent difference} = .4340 - 0.3363 / .4340 \times 100 = 22.5 \text{ percent}$$

RESULTS AND DISCUSSION

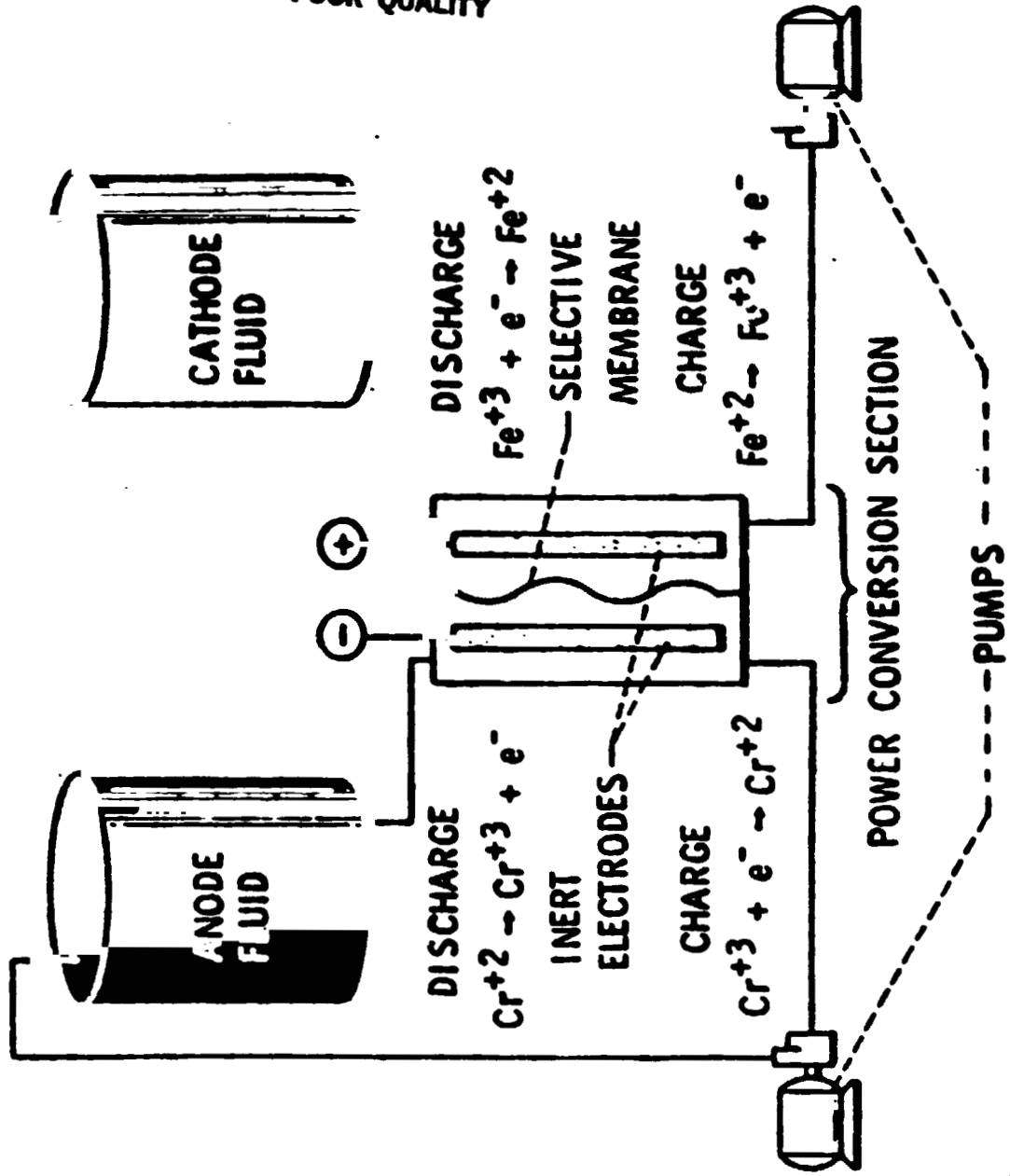
Results obtained from the computer and curve resolver are shown in tables 2 and 3. In table 2, two sets of data are given at different retaining values for each spectrum. The differences in concentrations appear to be minimal with the exception of spectra #43. In other cases, the number of equations used in the computation of concentrations remain constant regardless of the retaining value. Spectra 36 and 86 illustrate this behavior. This problem could very well be caused by low concentrations of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$. On the other hand, the curve resolver appears to have given more accurate data. Curve resolve data used in a similar study of chromium (III) complexes agrees with the accepted values ("Spectrophotometric Analysis of Aqueous Mixtures of Some Chromium (III) Complexes", Greg Stevens, May, 1983).

CONCLUSION

Table 4 compares the concentrations of the two methods. The discrepancy between these concentrations could have resulted from several factors. First of all, the temperature equilibrium data itself appears to be unreliable. Secondly, the computer analysis is inconsistent in its treatment of the data. The program may be unable to handle low concentrations of either species. Also, the selection of analytical wavelengths may have been poor. Consequently, it is desirable to choose wavelengths where one component absorbs strongly and the other weakly, or vice versa (2). The sharp slope of the curve analyzed could have also caused some discrepancy by giving inaccurate absorbance and wavelength readings. The curve resolver could have also added to this error. Since there are three variables for each of the four component curves, the probability that one can fit each curve perfectly remains quite low. As a result, we find that the computer analysis is not applicable to the data available.

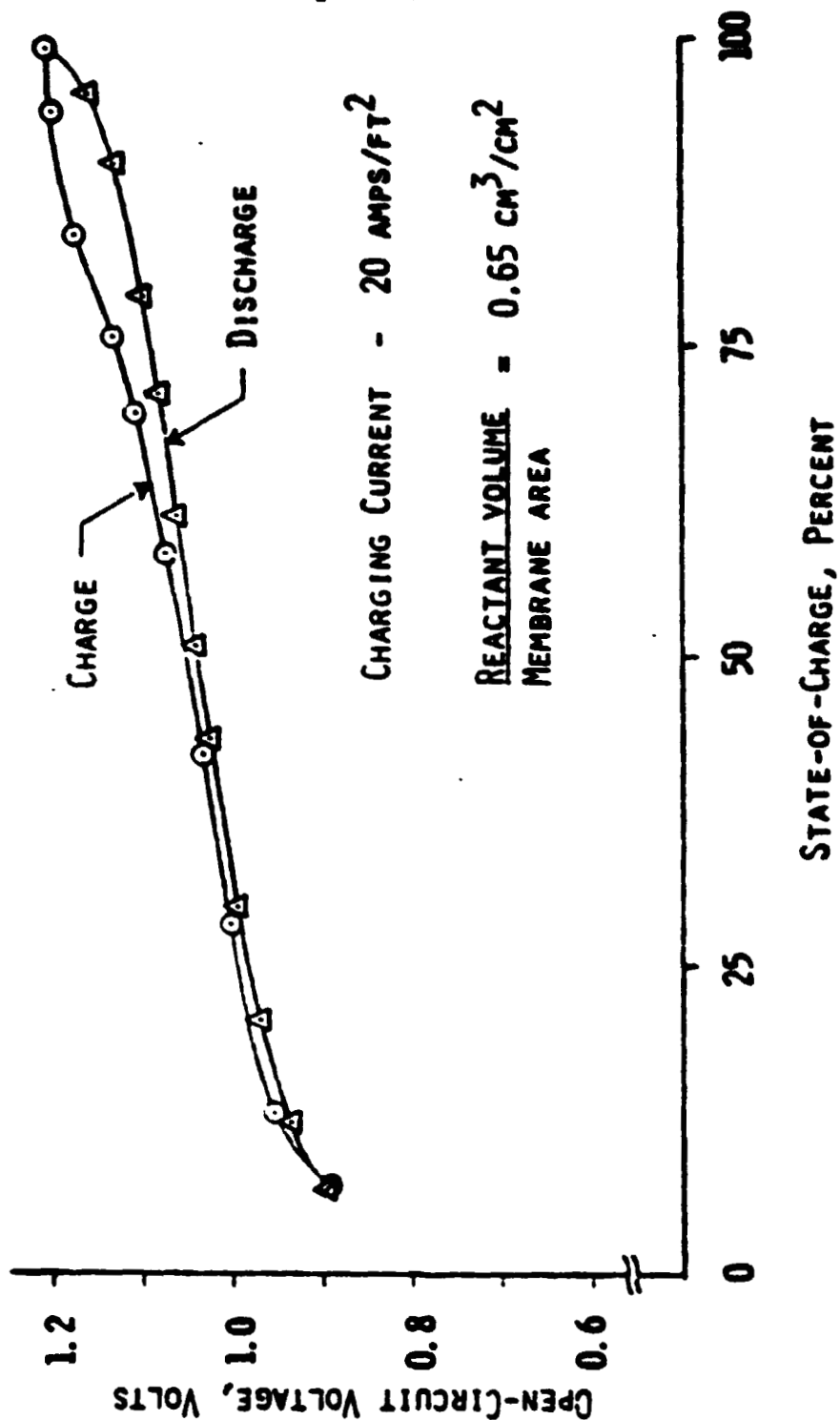
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FIGURE 1- PRINCIPLE OF OPERATION OF NASA-REDOX CONCEPT



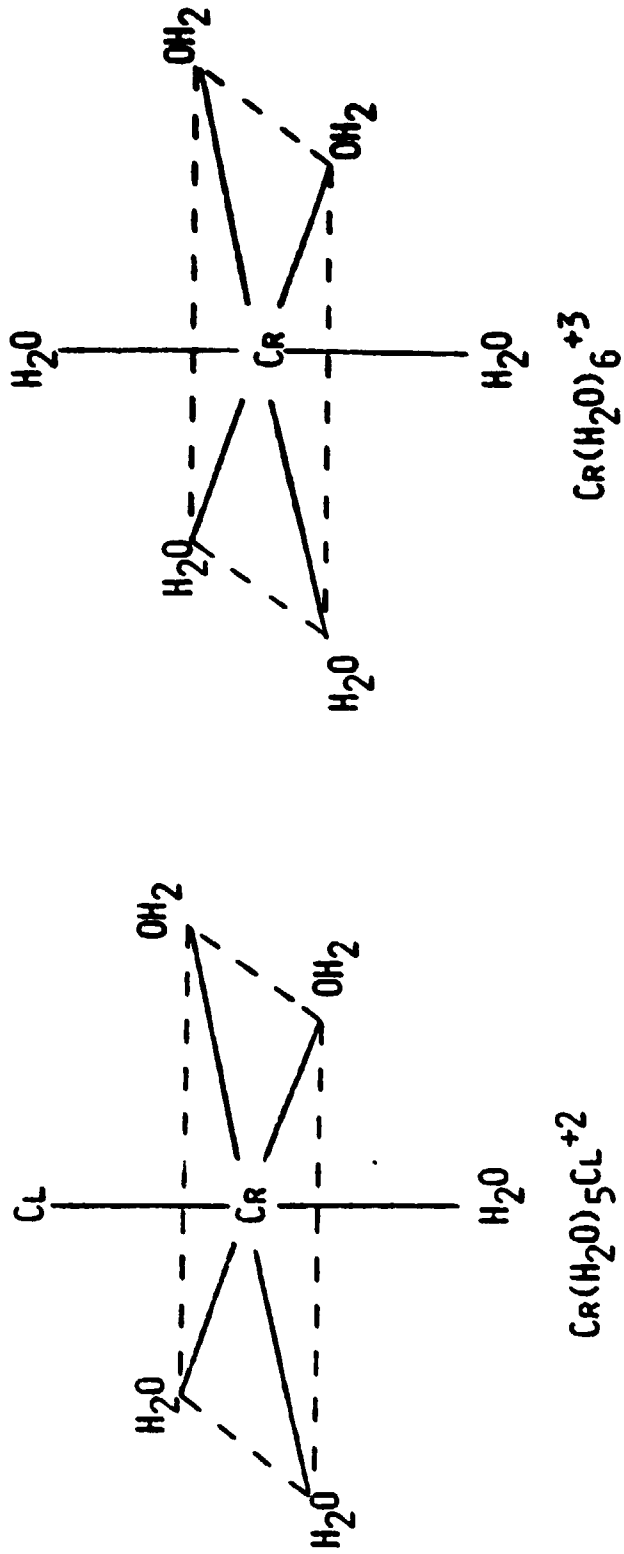
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FIGURE 2- OPEN-CIRCUIT VOLTAGE HYSTERESIS OF IRON/CHROMIUM REDOX CELL



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FIGURE 3- CR(III) COMPLEX IONS



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FIGURE. 4- SPECTRUM OF CHROMIUM REDOX SOLUTION

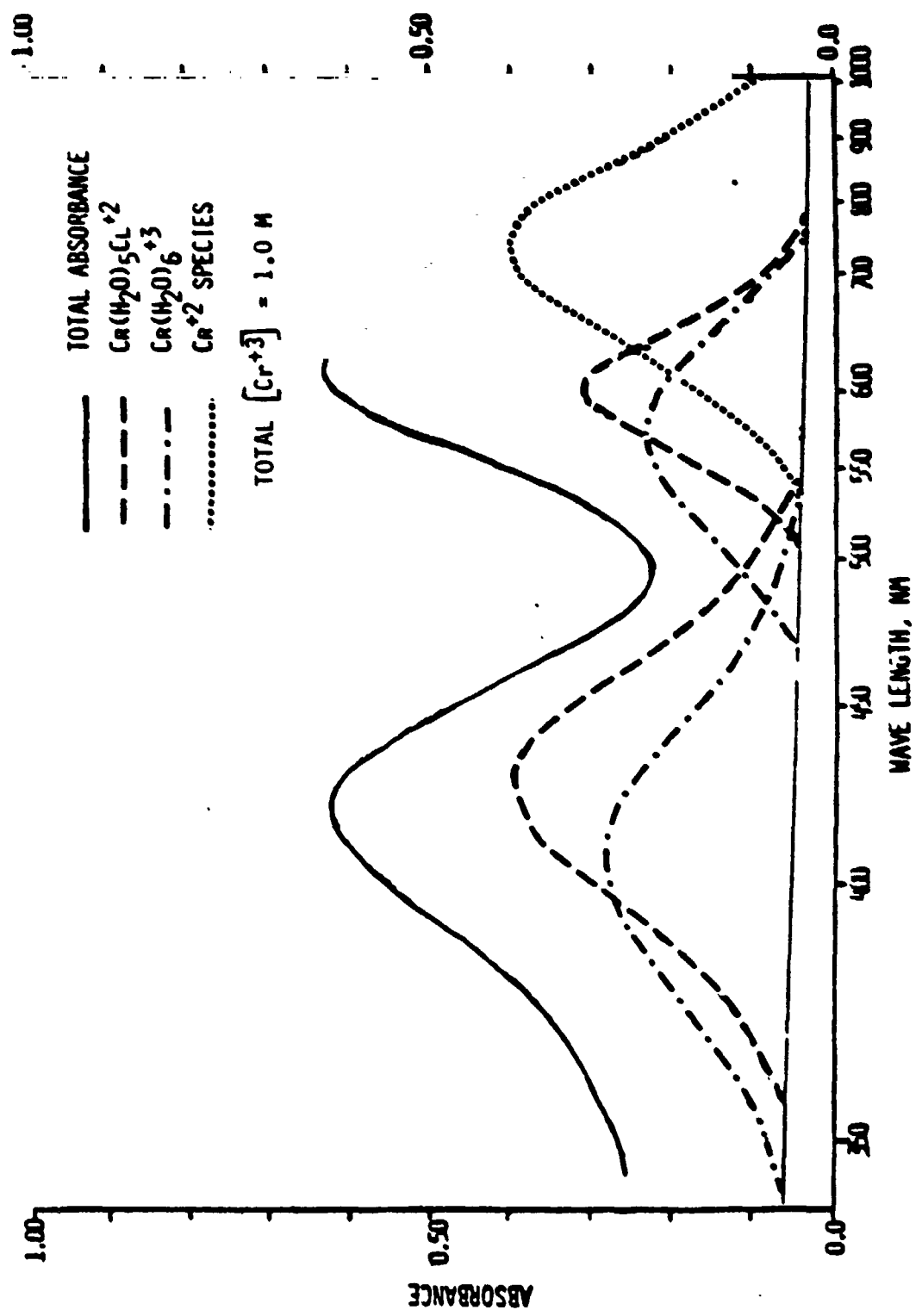
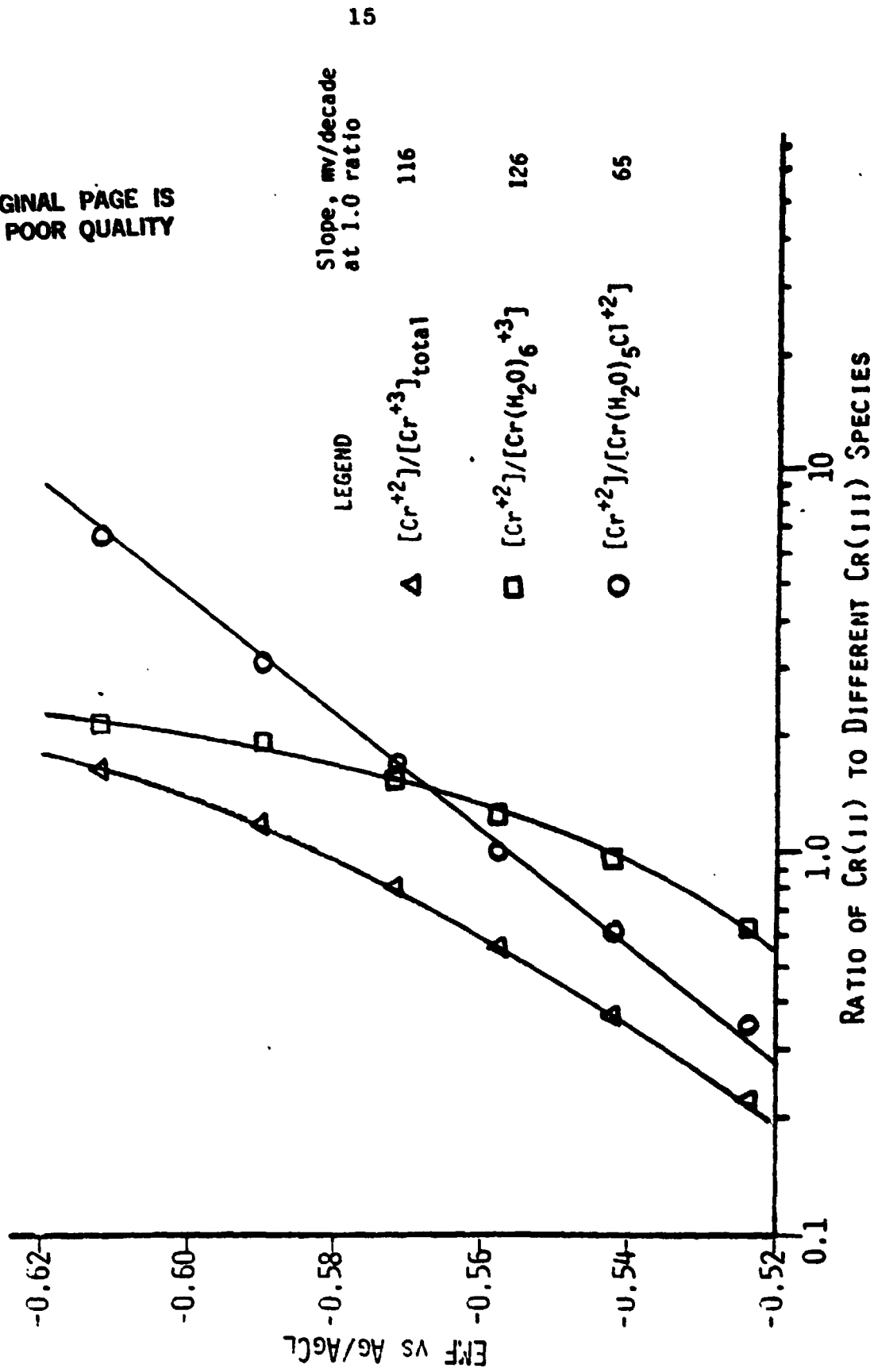


FIGURE. 5- POTENTIOMETRIC STUDIES

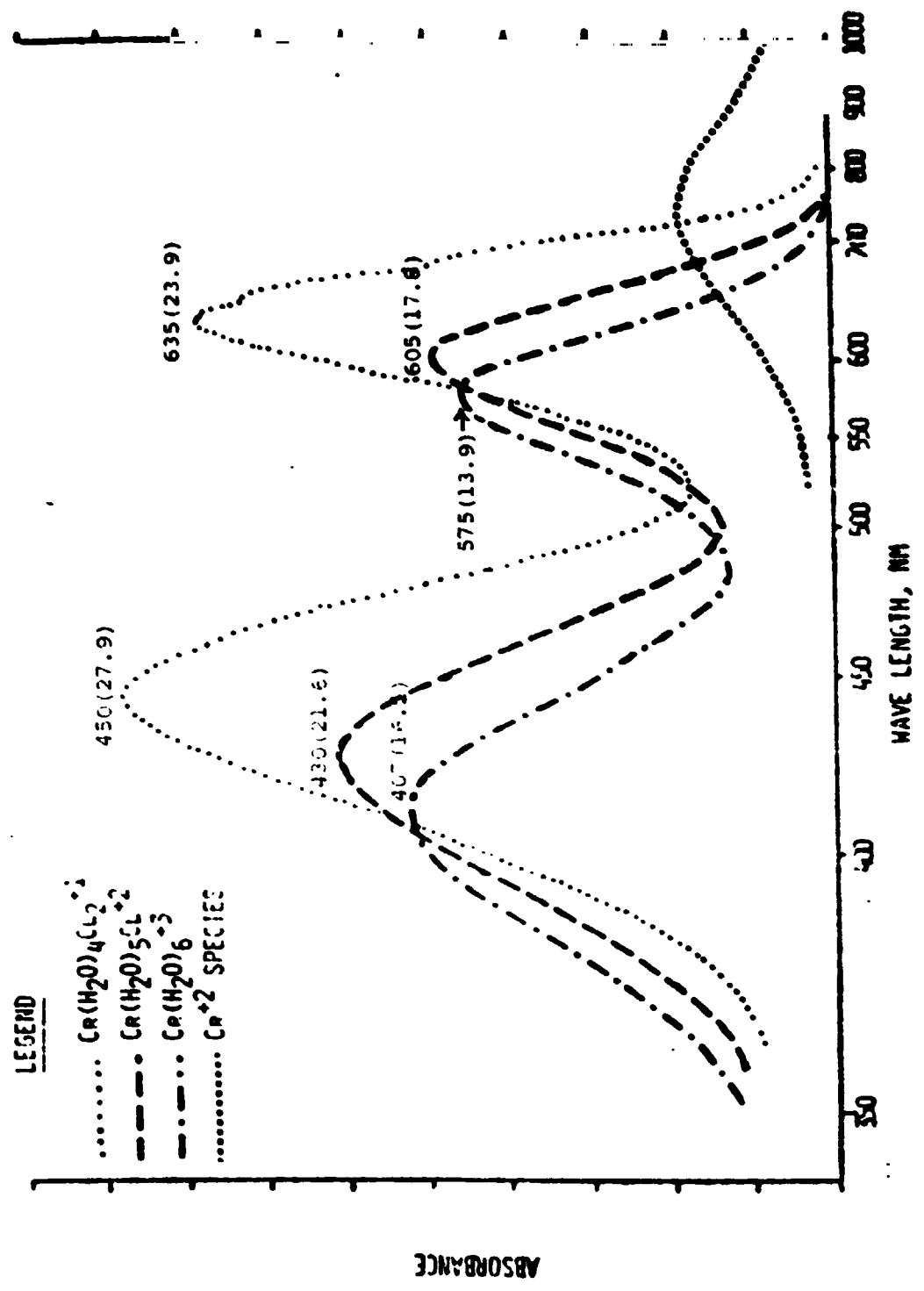
TEST OF NERNST EQUATION IN CHROMIUM
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FIGURE 6- SPECTRA OF CHROMIUM COMPLEX IONS



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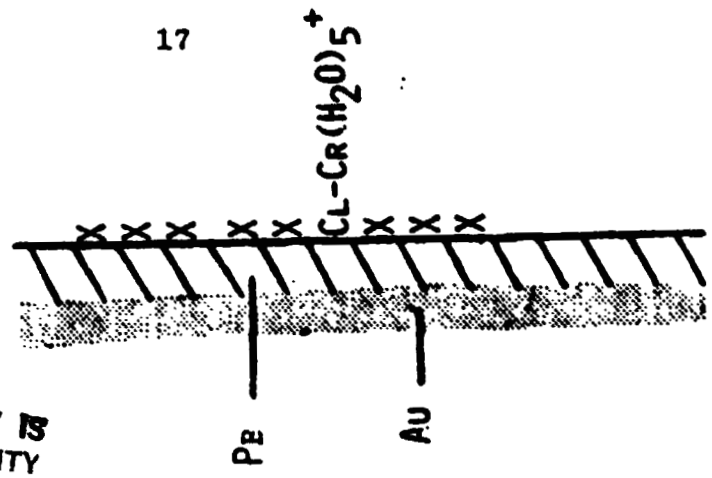
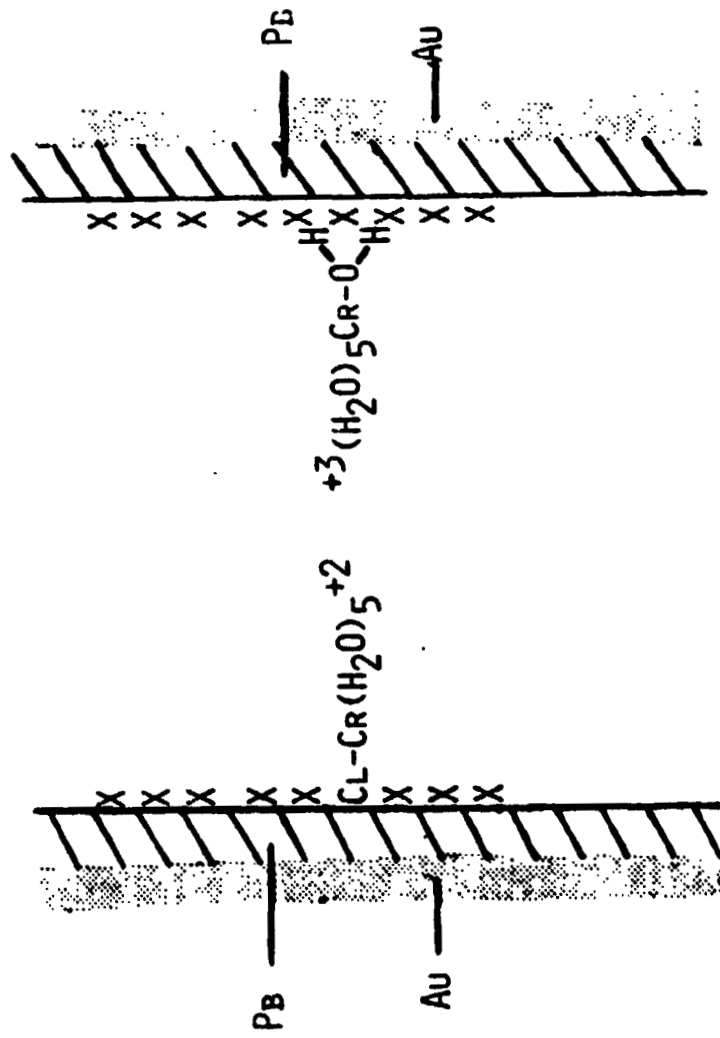


FIGURE. 7- ELECTRODE REACTION MECHANISMS



```

10 REM PROGRAM TO DETERMINE CONCENTRATIONS OF 2 COMPONENTS
20 REM IN MIXTURE FROM UV-VIS SPECTROSCOPY DATA
30 REM BY GREG STEVENS 3/83
40 REM
50 REM 1=0 TO 0 STEP .1=SET 0=FINISH
60 REM 1=0 TO 12=SET 1=0=INEXT
70 REM 1=0 TO 12=SET 1=1=INEXT
80 REM 1=0 TO 0 STEP .1=SET 1=20=INEXT
90 PRINT:PRINT "DETERMINATION OF CONCENTRATIONS OF TWO SPECIES IN A
100 PRINT:PRINT "SOLUTION USING UV-VIS SPECTROSCOPY DATA"
110 REM 1=0 TO 0=FINISH
120 PRINT:PRINT "HIT ANY KEY TO CONTINUE"
130 IF INKEY="" THEN GOTO 130
140 GOTO 3000
150 REM INPUT DATA
160 GOTO 3000
170 GOTO 3000
180 PRINT "ENTER THE NUMBER OF WAVELENGTHS FROM WHICH"
190 PRINT "DATA IS TAKEN"
200 INPUT I
210 IF I < 2 THEN GOTO 180 ELSE GOTO 220
220 PRINT "MINIMUM OF 2 ENTER AT LEAST 2 WAVELENGTHS"
230 GOTO 190
240 GOTO 3000
250 GOTO 3000
260 GOTO 3000
270 GOTO 3000
280 GOTO 3000
290 GOTO 3000
300 GOTO 3000
310 GOTO 3000
320 GOTO 3000
330 GOTO 3000
340 GOTO 3000
350 GOTO 3000
360 GOTO 3000
370 GOTO 3000
380 GOTO 3000
390 GOTO 3000
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480 GOTO 3000
490 GOTO 3000
500 GOTO 3000
510 GOTO 3000
520 GOTO 3000
530 GOTO 3000
540 GOTO 3000
550 GOTO 3000
560 GOTO 3000
570 GOTO 3000
580 GOTO 3000
590 GOTO 3000
600 GOTO 3000
610 GOTO 3000
620 GOTO 3000
630 GOTO 3000
640 GOTO 3000
650 GOTO 3000

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660 GOTO 1000
670 GOTO 1000
680 GOTO 1000
690 GOTO 1000
700 NEXT I
710 NEXT J
720 NEXT K
730 IF N=0 THEN GOTO 1000
740 NEXT L
750 NEXT M
760 NEXT N
770 NEXT O
780 NEXT P
790 NEXT Q
800 REM PRINT OUTPUT CONCENTRATIONS
810 LPRINT "LPRINT"
820 LPRINT "THE CONCENTRATION OF THE FIRST SPECIES IS "Y1" MOLAR"
830 LPRINT " "
840 LPRINT "THE CONCENTRATION OF THE SECOND SPECIES IS "Y2" MOLAR"
850 LPRINT "LPRINT"
860 LPRINT "FIRST SPECIES STANDARD DEVIATION IS "S1" LPRINT USING #0:10
870 LPRINT "SECOND SPECIES STANDARD DEVIATION IS "S2" LPRINT USING #0:10
880 LPRINT " "
890 LPRINT "FIRST SPECIES RELATIVE AVERAGE DEVIATION IS "R1" LPRINT USING #0:10
900 LPRINT "SECOND SPECIES RELATIVE AVERAGE DEVIATION IS "R2" LPRINT USING #0:10
910 REM PRINT OUT COMPUTED CONCENTRATIONS AND THEIR
920 REM STANDARD DEVIATION AND RELATIVE AVERAGE DEVIATION
930 LPRINT "LPRINT"
940 LPRINT " "DATA" LPRINT " "
950 LPRINT "CONCENTRATION #1" "CONCENTRATION #2"
960 LPRINT " "
970 NEXT I
980 NEXT J
990 NEXT K
1000 LPRINT " "
1010 NEXT L
1020 NEXT M
1030 NEXT N
1040 NEXT O
1050 NEXT P
1060 NEXT Q
1070 NEXT R
1080 NEXT S
1090 NEXT T
1100 NEXT U
1110 NEXT V
1120 NEXT W
1130 NEXT X
1140 NEXT Y
1150 NEXT Z
1160 NEXT AA
1170 NEXT AB
1180 NEXT AC
1190 NEXT AD
1200 NEXT AE
1210 NEXT AF
1220 NEXT AG
1230 NEXT AH
1240 NEXT AI
1250 NEXT AJ
1260 NEXT AK
1270 NEXT AL
1280 NEXT AM
1290 NEXT AN
1300 NEXT AO
1310 NEXT AP
1320 NEXT AQ
1330 NEXT AR
1340 NEXT AS
1350 NEXT AT
1360 NEXT AU
1370 NEXT AV
1380 NEXT AW
1390 NEXT AX
1400 NEXT AY
1410 NEXT AZ
1420 NEXT BA
1430 NEXT BB
1440 NEXT BC
1450 NEXT BD
1460 NEXT BE
1470 NEXT BF
1480 NEXT BG
1490 NEXT BH
1500 NEXT BI
1510 NEXT BJ
1520 NEXT BK
1530 NEXT BL
1540 NEXT BM
1550 NEXT BN
1560 NEXT BO
1570 NEXT BP
1580 NEXT BQ
1590 NEXT BR
1600 NEXT BS
1610 NEXT BT
1620 NEXT BU
1630 NEXT BV
1640 NEXT BW
1650 NEXT BX
1660 NEXT BY
1670 NEXT BZ
1680 NEXT CA
1690 NEXT CB
1700 NEXT CC
1710 NEXT CD
1720 NEXT CE
1730 NEXT CF
1740 NEXT CG
1750 NEXT CH
1760 NEXT CI
1770 NEXT CJ
1780 NEXT CK
1790 NEXT CL
1800 NEXT CM
1810 NEXT CN
1820 NEXT CO
1830 NEXT CP
1840 NEXT CQ
1850 NEXT CR
1860 NEXT CS
1870 NEXT CT
1880 NEXT CU
1890 NEXT CV
1900 NEXT CW
1910 NEXT CX
1920 NEXT CY
1930 NEXT CZ
1940 NEXT DA
1950 NEXT DB
1960 NEXT DC
1970 NEXT DD
1980 NEXT DE
1990 NEXT DF
2000 NEXT DG
2010 NEXT DH
2020 NEXT DI
2030 NEXT DJ
2040 NEXT DK
2050 NEXT DL
2060 NEXT DM
2070 NEXT DN
2080 NEXT DO
2090 NEXT DP
2100 NEXT DQ
2110 NEXT DR
2120 NEXT DS
2130 NEXT DT
2140 NEXT DU
2150 NEXT DV
2160 NEXT DW
2170 NEXT DX
2180 NEXT DY
2190 NEXT DZ
2200 NEXT EA
2210 NEXT EB
2220 NEXT EC
2230 NEXT ED
2240 NEXT EE
2250 NEXT EF
2260 NEXT EG
2270 NEXT EH
2280 NEXT EI
2290 NEXT EJ
2300 NEXT EK
2310 NEXT EL
2320 NEXT EM
2330 NEXT EN
2340 NEXT EO
2350 NEXT EP
2360 NEXT EQ
2370 NEXT ER
2380 NEXT ES
2390 NEXT ET
2400 NEXT EU
2410 NEXT EV
2420 NEXT EW
2430 NEXT EX
2440 NEXT EY
2450 NEXT EZ
2460 NEXT FA
2470 NEXT FB
2480 NEXT FC
2490 NEXT FD
2500 NEXT FE
2510 NEXT FF
2520 NEXT FG
2530 NEXT FH
2540 NEXT FI
2550 NEXT FJ
2560 NEXT FK
2570 NEXT FL
2580 NEXT FM
2590 NEXT FN
2600 NEXT FO
2610 NEXT FP
2620 NEXT FQ
2630 NEXT FR
2640 NEXT FS
2650 NEXT FT
2660 NEXT FU
2670 NEXT FV
2680 NEXT FW
2690 NEXT FX
2700 NEXT FY
2710 NEXT FZ
2720 NEXT GA
2730 NEXT GB
2740 NEXT GC
2750 NEXT GD
2760 NEXT GE
2770 NEXT GF
2780 NEXT GG
2790 NEXT GH
2800 NEXT GI
2810 NEXT GJ
2820 NEXT GK
2830 NEXT GL
2840 NEXT GM
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2890 NEXT GR
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2970 NEXT GZ
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3000 NEXT HC
3010 NEXT HD
3020 NEXT HE
3030 NEXT HF
3040 NEXT HG
3050 NEXT HH
3060 NEXT HI
3070 NEXT HJ
3080 NEXT HK
3090 NEXT HL
3100 NEXT HM
3110 NEXT HN
3120 NEXT HO
3130 NEXT HP
3140 NEXT HQ
3150 NEXT HR
3160 NEXT HS
3170 NEXT HT
3180 NEXT HU
3190 NEXT HV
3200 NEXT HW
3210 NEXT HX
3220 NEXT HY
3230 NEXT HZ
3240 NEXT IA
3250 NEXT IB
3260 NEXT IC
3270 NEXT ID
3280 NEXT IE
3290 NEXT IF
3300 NEXT IG
3310 NEXT IH
3320 NEXT II
3330 NEXT IJ
3340 NEXT IK
3350 NEXT IL
3360 NEXT IM
3370 NEXT IN
3380 NEXT IO
3390 NEXT IP
3400 NEXT IQ
3410 NEXT IR
3420 NEXT IS
3430 NEXT IT
3440 NEXT IU
3450 NEXT IV
3460 NEXT IW
3470 NEXT IX
3480 NEXT IY
3490 NEXT IZ
3500 NEXT JA
3510 NEXT JB
3520 NEXT JC
3530 NEXT JD
3540 NEXT JE
3550 NEXT JF
3560 NEXT JG
3570 NEXT JH
3580 NEXT JI
3590 NEXT JJ
3600 NEXT JK
3610 NEXT JL
3620 NEXT JM
3630 NEXT JN
3640 NEXT JO
3650 NEXT JP
3660 NEXT JQ
3670 NEXT JR
3680 NEXT JS
3690 NEXT JT
3700 NEXT JU
3710 NEXT JV
3720 NEXT JW
3730 NEXT JX
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1490 NEXT CT
1491 NEXT CU
1492 NEXT CV
1493 NEXT CW
1494 NEXT CX
1495 NEXT CY
1496 NEXT CZ
1497 NEXT DA
1498 NEXT DB
1499 NEXT DC
1500 NEXT DE
1501 NEXT DF
1502 NEXT DG
1503 NEXT DH
1504 NEXT DI
1505 NEXT DJ
1506 NEXT DK
1507 NEXT DL
1508 NEXT DM
1509 NEXT DN
1510 NEXT DO
1511 NEXT DP
1512 NEXT DQ
1513 NEXT DR
1514 NEXT DS
1515 NEXT DT
1516 NEXT DU
1517 NEXT DV
1518 NEXT DW
1519 NEXT DX
1520 NEXT DY
1521 NEXT DZ
1522 NEXT EA
1523 NEXT EB
1524 NEXT EC
1525 NEXT ED
1526 NEXT EE
1527 NEXT EF
1528 NEXT EG
1529 NEXT EH
1530 NEXT EI
1531 NEXT EJ
1532 NEXT EK
1533 NEXT EL
1534 NEXT EM
1535 NEXT EN
1536 NEXT EO
1537 NEXT EP
1538 NEXT EQ
1539 NEXT ER
1540 NEXT ES
1541 NEXT ET
1542 NEXT EU
1543 NEXT EV
1544 NEXT EW
1545 NEXT EX
1546 NEXT EY
1547 NEXT EZ
1548 NEXT FA
1549 NEXT FB
1550 NEXT FC
1551 NEXT FD
1552 NEXT FE
1553 NEXT FF
1554 NEXT FG
1555 NEXT FH
1556 NEXT FI
1557 NEXT FJ
1558 NEXT FK
1559 NEXT FL
1560 NEXT FM
1561 NEXT FN
1562 NEXT FO
1563 NEXT FP
1564 NEXT FQ
1565 NEXT FR
1566 NEXT FS
1567 NEXT FT
1568 NEXT FU
1569 NEXT FV
1570 NEXT FW
1571 NEXT FX
1572 NEXT FY
1573 NEXT FZ
1574 NEXT GA
1575 NEXT GB
1576 NEXT GC
1577 NEXT GD
1578 NEXT GE
1579 NEXT GF
1580 NEXT GG
1581 NEXT GH
1582 NEXT GI
1583 NEXT GJ
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1585 NEXT GL
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1587 NEXT GN
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1589 NEXT GP
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1593 NEXT GT
1594 NEXT GU
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1599 NEXT GZ
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1602 NEXT HC
1603 NEXT HD
1604 NEXT HE
1605 NEXT HF
1606 NEXT HG
1607 NEXT HH
1608 NEXT HI
1609 NEXT HJ
1610 NEXT HK
1611 NEXT HL
1612 NEXT HM
1613 NEXT HN
1614 NEXT HO
1615 NEXT HP
1616 NEXT HQ
1617 NEXT HR
1618 NEXT HS
1619 NEXT HT
1620 NEXT HU
1621 NEXT HV
1622 NEXT HW
1623 NEXT HX
1624 NEXT HY
1625 NEXT HZ
1626 NEXT IA
1627 NEXT IB
1628 NEXT IC
1629 NEXT ID
1630 NEXT IE
1631 NEXT IF
1632 NEXT IG
1633 NEXT IH
1634 NEXT II
1635 NEXT IJ
1636 NEXT IK
1637 NEXT IL
1638 NEXT IM
1639 NEXT IN
1640 NEXT IO
1641 NEXT IP
1642 NEXT IQ
1643 NEXT IR
1644 NEXT IS
1645 NEXT IT
1646 NEXT IU
1647 NEXT IV
1648 NEXT IW
1649 NEXT IX
1650 NEXT IY
1651 NEXT IZ
1652 NEXT JA
1653 NEXT JB
1654 NEXT JC
1655 NEXT JD
1656 NEXT JE
1657 NEXT JF
1658 NEXT JG
1659 NEXT JH
1660 NEXT JI
1661 NEXT JJ
1662 NEXT JK
1663 NEXT JL
1664 NEXT JM
1665 NEXT JN
1666 NEXT JO
1667 NEXT JP
1668 NEXT JQ
1669 NEXT JR
1670 NEXT JS
1671 NEXT JT
1672 NEXT JU
1673 NEXT JV
1674 NEXT JW
1675 NEXT JX
1676 NEXT JY
1677 NEXT JZ
1678 NEXT KA
1679 NEXT KB
1680 NEXT KC
1681 NEXT KD
1682 NEXT KE
1683 NEXT KF
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1685 NEXT KH
1686 NEXT KI
1687 NEXT KJ
1688 NEXT KK
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1691 NEXT KN
1692 NEXT KO
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1719 NEXT LQ
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1722 NEXT LT
1723 NEXT LU
1724 NEXT LV
1725 NEXT LW
1726 NEXT LX
1727 NEXT LY
1728 NEXT LZ
1729 NEXT MA
1730 NEXT MB
1731 NEXT MC
1732 NEXT MD
1733 NEXT ME
1734 NEXT MF
1735 NEXT MG
1736 NEXT MH
1737 NEXT MI
1738 NEXT MJ
1739 NEXT MK
1740 NEXT ML
1741 NEXT MM
1742 NEXT MN
1743 NEXT MO
1744 NEXT MP
1745 NEXT MQ
1746 NEXT MR
1747 NEXT MS
1748 NEXT MT
1749 NEXT MU
1750 NEXT MV
1751 NEXT MW
1752 NEXT MX
1753 NEXT MY

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2000 REM LINES 2000-2100 ELIMINATE EFFERESCENT CONCENTRATION VALUES
2005 L=0
2010 N=2:R=0:R1=0:R2=0
2020 FOR I=1 TO E
2030 FOR J=1 TO E
2040 IF (A(I,J)-C(I,J))>.05 THEN R=R+1:R1=R1+1:R2=R2+1:GOTO 2005
2050 I=I+1
2060 IF I>E THEN J=J+1
2070 IF J>E THEN R=R+1:R1=R1+1:R2=R2+1
2080 IF L=9 THEN GOSUB 3000
2090 NEXT J
2100 N=N+1
2110 IF L=(D-1) THEN GOTO 2115
2120 NEXT I
2130 N=N+1
2145 IF N=0 THEN N=1
2150 Y=S1/N
2160 Y=S2/N
2175 N=N+1
2180 Y=INT(Y*10000+.5)/10000
2190 Y=INT(Y*10000+.5)/10000
2200 L=L+1
2210 IF L=10 THEN GOTO 2190
2220 GOTO 2010
2230 RETURN
3000 REM INPUT TITLE
3005 CLEAR 64
3010 INPUT "ENTER THE TITLE: "T$
3020 LPRINT T$
3030 LPRINT "LPRINT"
3040 GOTO 170
4000 REM COMPUTE ED AND RAD FOR REMAINING VALUES
4020 SD(1,1)=(C(1,1)-Y)*2
4030 SD(2,1)=SD(1,1)+SD(2,1)
4040 RAD(1,1)=ABS(C(1,1)-Y)
4050 RAD(2,1)=RAD(1,1)+RAD(2,1)
4060 SD(1,2)=(C(1,2)-Y)*2
4070 SD(2,2)=SD(1,2)+SD(2,2)
4080 RAD(1,2)=ABS(C(1,2)-Y)
4090 RAD(2,2)=RAD(1,2)+RAD(2,2)
4100 N=N+1
4110 IF N=2 THEN N=2
4120 IF X=0 OR Y=0 THEN X=1:Y=1
4130 F(1)=(SD(2,1)/(N-1))*5
4140 G(1)=(RAD(2,1)/(N-1))*100
4150 F(2)=(SD(2,2)/(N-1))*5
4160 G(2)=(RAD(2,2)/(N-1))*100
4170 N=N+1
4180 RETURN
5000 PRINT "DO YOU WISH TO USE THE SPECIFIED WAVELENGTHS FOR"
5010 PRINT "CHROMIUM ANALYSIS--652,629,592,556,532,460,442,416."
5020 INPUT "YES AND 370"K$
5030 IF K$="YES" THEN GOTO 6040 ELSE RETURN
6040 CLS
6050 FOR I=1 TO E
6070 READ W(1),W(2),W(3),W(4),W(5),W(6),W(7),W(8)
6080 PRINT "ENTER ABSORBANCE AT WAVELENGTH" W(I)
6090 INPUT A(I)
6110 NEXT I
6120 PRINT "PLEASE WAIT"
6130 GOTO 460
6200 DATA 652,629,592,556,532,460,442,416
6300 DATA 256,6,93,12,81,1,532,5,84,8,95,1,440,13,21,5,25,1
6400 DATA 440,15,9,18,55,1,416,19,62,16,93,1,359,7,78,16,16
6500 DATA 1,270,2,58,11,93,1
6600 END

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Table 2.- Computer Output for Spectra Obtained From Equilibrium Temperature Study

<u>Spectra #</u>	<u>Number of equations used</u>	<u>Retaining value</u>	<u>C_P(mol/l)</u>	<u>C_H(mol/l)</u>	<u>SD_P</u>	<u>SD_H</u>	<u>RAD_P(%)</u>	<u>RAD_H(%)</u>
88	17	0.25	0.6135	0.3377	0.050	0.029	6.64	7.31
88	25	0.50	0.6389	0.3274	0.082	0.073	9.32	16.17
36	2	0.25	0.8103	0.0761	0.018	0.015	3.07	27.66
36	5	0.75	0.8190	0.0667	0.028	0.033	3.20	45.48
52	18	0.25	0.5607	0.3245	0.035	0.039	5.16	11.04
52	34	0.50	0.5606	0.3483	0.088	0.088	11.53	21.67
86	2	0.25	0.7720	0.0699	0.013	0.015	2.31	29.59
86	2	0.75	0.7720	0.0699	0.013	0.015	2.31	29.59
82	18	0.25	0.6207	0.3363	0.048	0.033	6.38	7.77
82	26	0.50	0.6436	0.3262	0.081	0.074	9.19	16.87
43	5	0.25	0.8753	0.0756	0.091	0.006	9.25	7.00
43	38	0.75	0.7668	0.1870	0.072	0.062	6.96	24.21
66	20	0.25	0.5212	0.3602	0.036	0.047	5.93	11.62
66	33	0.50	0.4962	0.4118	0.071	0.101	11.54	21.04
92	18	0.25	0.5275	0.3989	0.047	0.034	6.33	6.88
92	33	0.50	0.5171	0.1213	0.079	0.102	11.87	20.15

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OF POOR QUALITYC_P = concentration of Cr(H₂O)₅Cl⁺²C_H = concentration of Cr(H₂O)₆⁺³SD_P = standard deviation of Cr(H₂O)₅Cl⁺²SD_H = standard deviation of Cr(H₂O)₆⁺³RAD_P = relative average deviation of Cr(H₂O)₅Cl⁺²RAD_H = relative average deviation of Cr(H₂O)₆⁺³

Table 3. - Curve Resolve Data for Spectra Obtained from
Equilibrium Temperature Study

Spectra #	$C_p(\text{mol/l})$	$C_H(\text{mol/l})$	A_{p1}	A_{p2}	A_{H1}	A_{H2}
88	0.5187	0.3825	0.930	1.112	0.540	0.606
36	0.7052	0.1503	1.258	1.520	0.194	0.259
52	0.2900	0.3710	0.888	1.039	0.522	0.590
86	0.5987	0.5660	1.087	1.267	0.540	0.592
82	0.4927	0.4340	0.897	1.040	0.597	0.706
43	0.7485	0.1136	1.351	1.594	0.150	0.192
66	0.3794	0.4900	0.684	0.809	0.680	0.790
92	0.3921	0.5018	0.688	0.859	0.705	0.799

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A_{p1} = absorbance of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ at first peak
 A_{p2} = absorbance of $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$ at second peak
 A_{H1} = absorbance of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ at first peak
 A_{H2} = absorbance of $\text{Cr}(\text{H}_2\text{O})_6^{+3}$ at second peak

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Table 4.- Comparison of Data Obtained From
Computer and Curve Resolver

<u>Spectra #</u>	<u>Computer</u>		<u>Resolver</u>	
	<u>C_p(mol/l)</u>	<u>C_H(mol/l)</u>	<u>C_p(mol/l)</u>	<u>C_H(mol/l)</u>
88	0.6135	0.3377	0.5187	0.3825
36	0.8103	0.0761	0.7052	0.1503
52	0.5606	0.3483	0.4900	0.3710
86	0.7720	0.0699	0.5987	0.5660
82	0.6207	0.3363	0.4927	0.4340
43	0.7668	0.1870	0.7485	0.1136
66	0.4962	0.4118	0.3794	0.4900
92	0.5171	0.4213	0.3921	0.5018

FIGURE 8- SPECTRA # 82

1M CrCl₂ in 1.0N HCl
 0-1 scale, med. speed
 20mv range
 25ml sample @ 26°C for 4hrs.

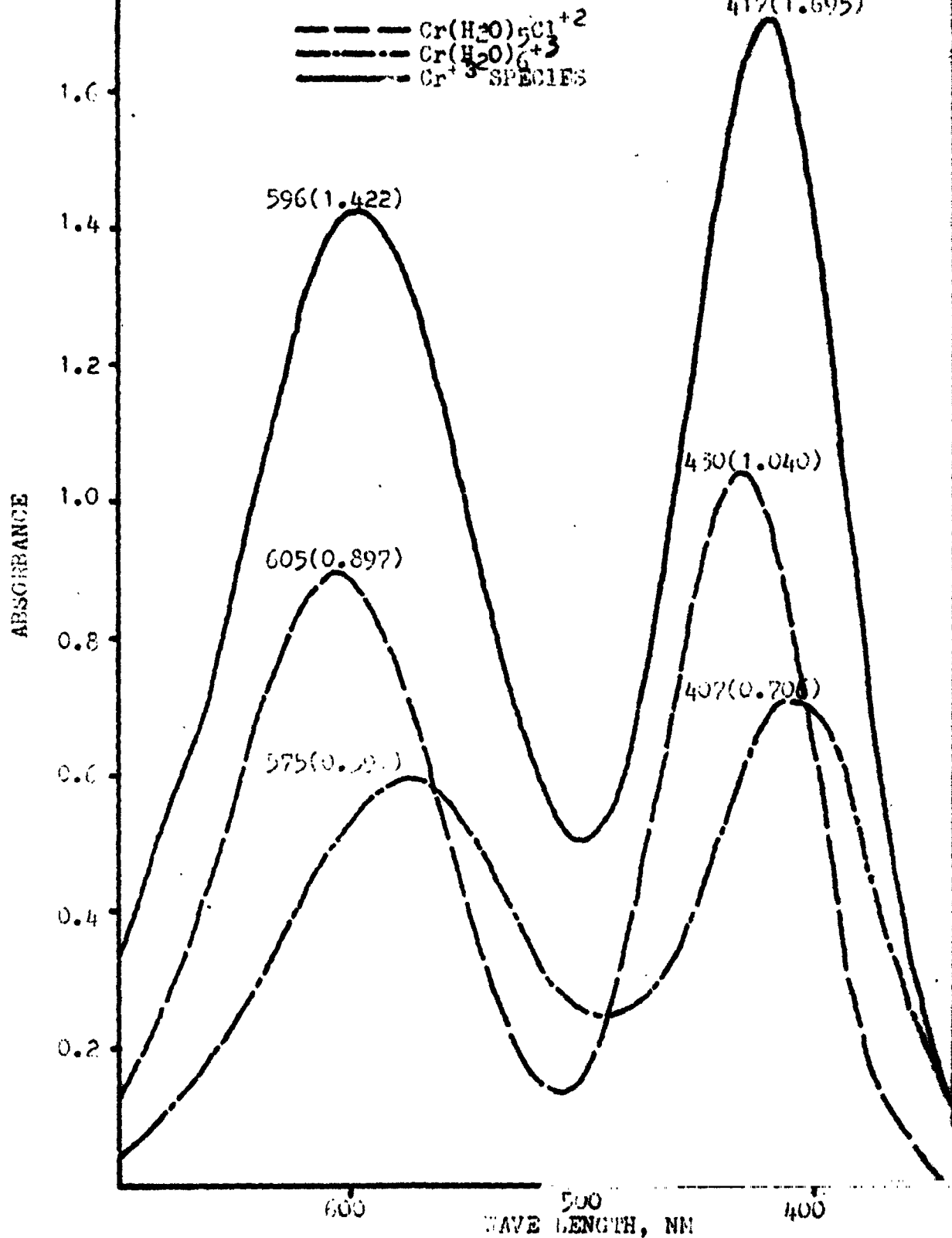


FIGURE 9- SPECTRA #43

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1M CrCl_3 in 1.0N HCl
 0-1 scale, med. speed
 20mv range
 25 ml sample @ 40°C for 24hrs.

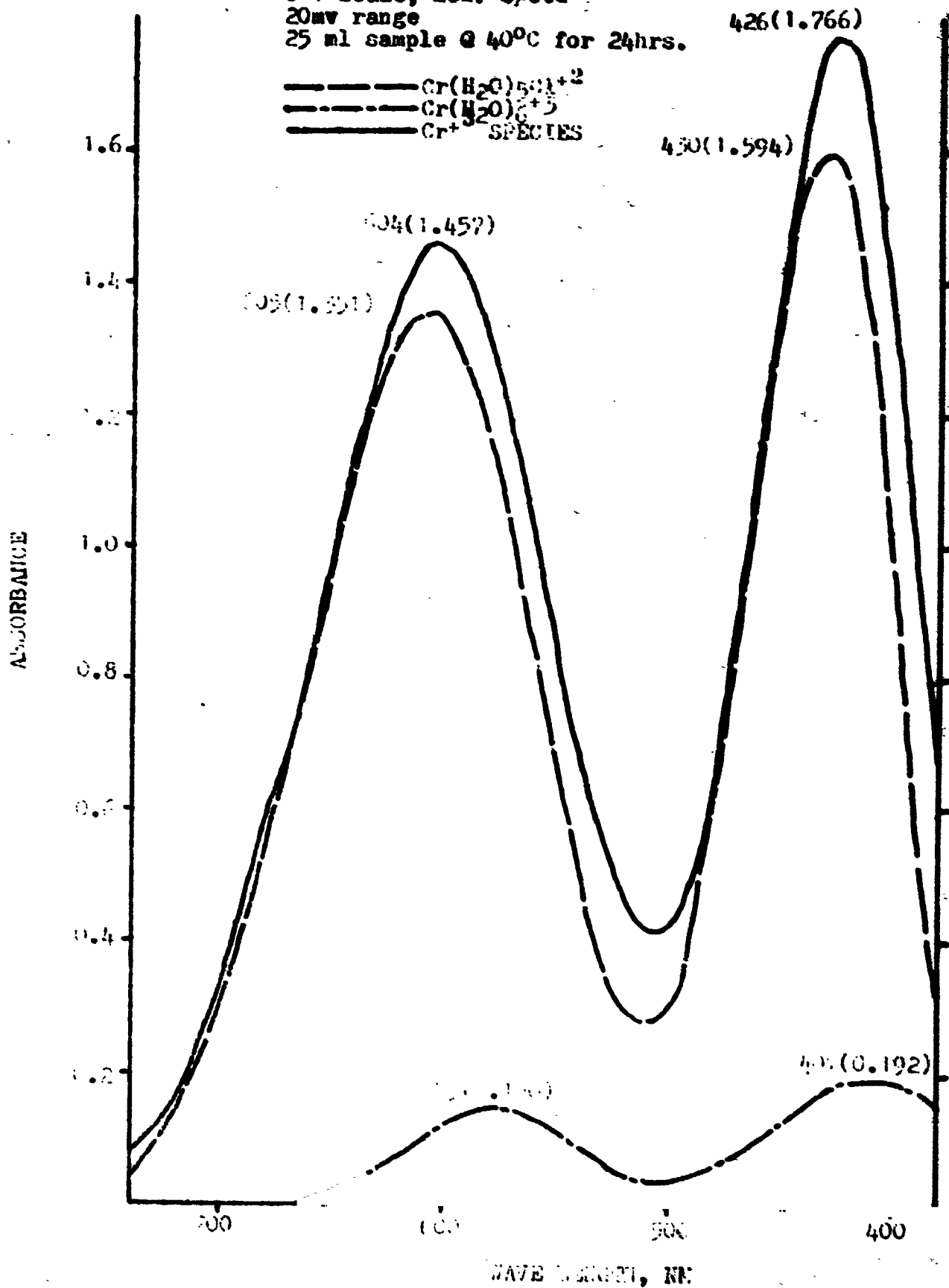


FIGURE 10- SPECTRA #66

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1% CrCl_3 in 1.0N HCl
 0-1 scale, med. speed
 20mv range
 25ml sample @ 55°C for 24hrs.

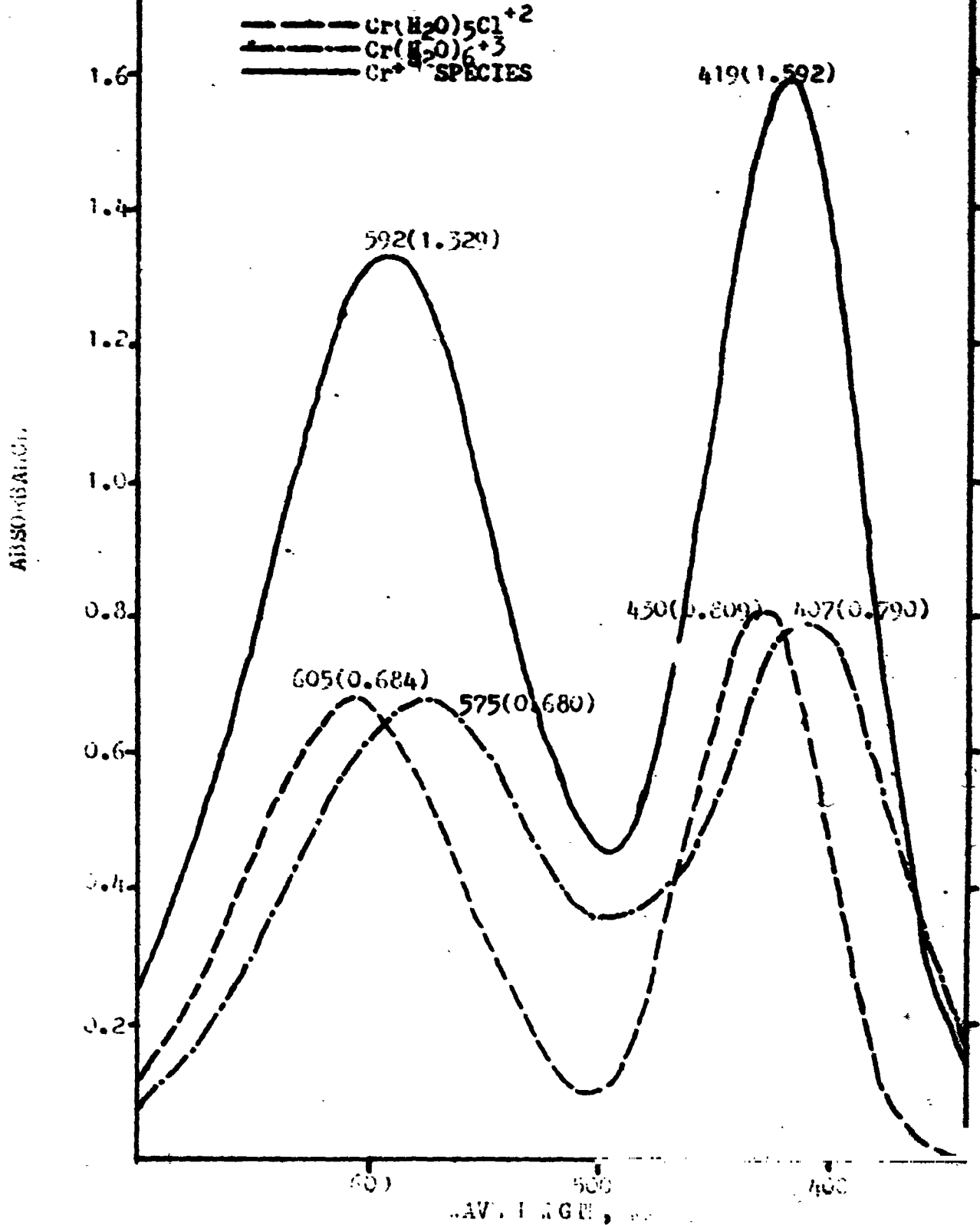
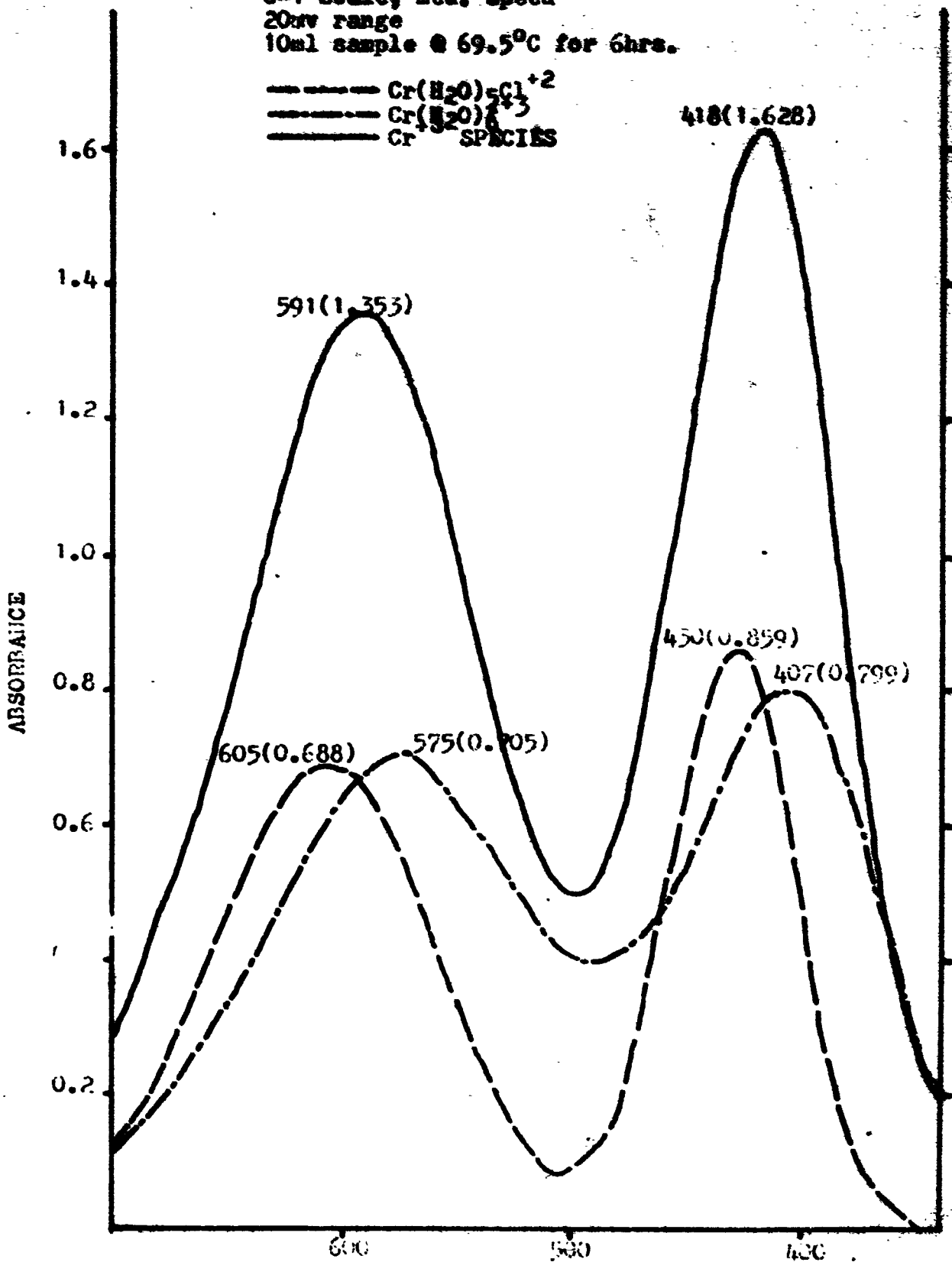


FIGURE 11. - SPECTRA #92

CRONEX FILM IS
OF POOR QUALITY

1% CrCl₃ in 1.0N HCl
0-1 scale, med. speed
20mv range
10ml sample @ 69.5°C for 6hrs.

----- Cr(H₂O)₅Cl⁺²
- - - - - Cr(H₂O)₆⁺³
————— Cr⁺³ SPECIES



WAVELENGTH, mμ

FIGURE. 12- SPECTRA #88

ORIGINAL PAGE IS
OF POOR QUALITY

1M CrCl_3 in 2.0N HCl
 0-1 scale, med. speed
 20mv range
 25ml sample @ 20°C for 4hrs. 418(1.672)

— — — $\text{Cr}(\text{H}_2\text{O})_5\text{Cl}^{+2}$
 - - - - $\text{Cr}(\text{H}_2\text{O})_4^{+3}$
 — — — Cr^{+3} SPECIES

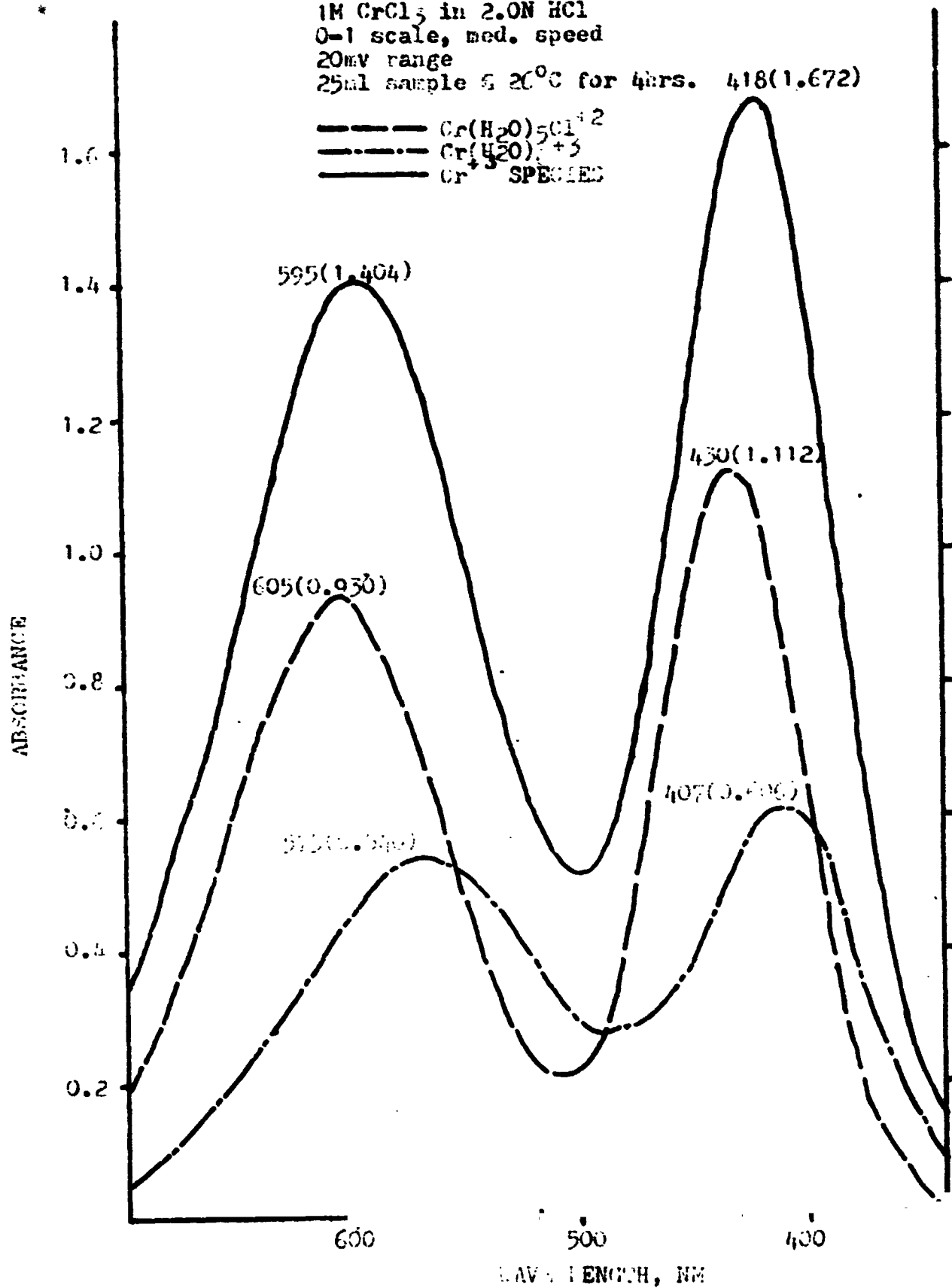


FIGURE 13- SPECTRA # 36

ORIGINAL FILE IN
OF FOUR QUALITY

1M CrCl₃ in 2.0N HCl
0-1 scale, med. speed
20mv range
25ml sample @ 40°C for 24hrs.

— — — — — Cr(H₂O)₅Cl²⁺
- - - - - Cr(H₂O)₆³⁺
————— Cr³⁺ SPECIES

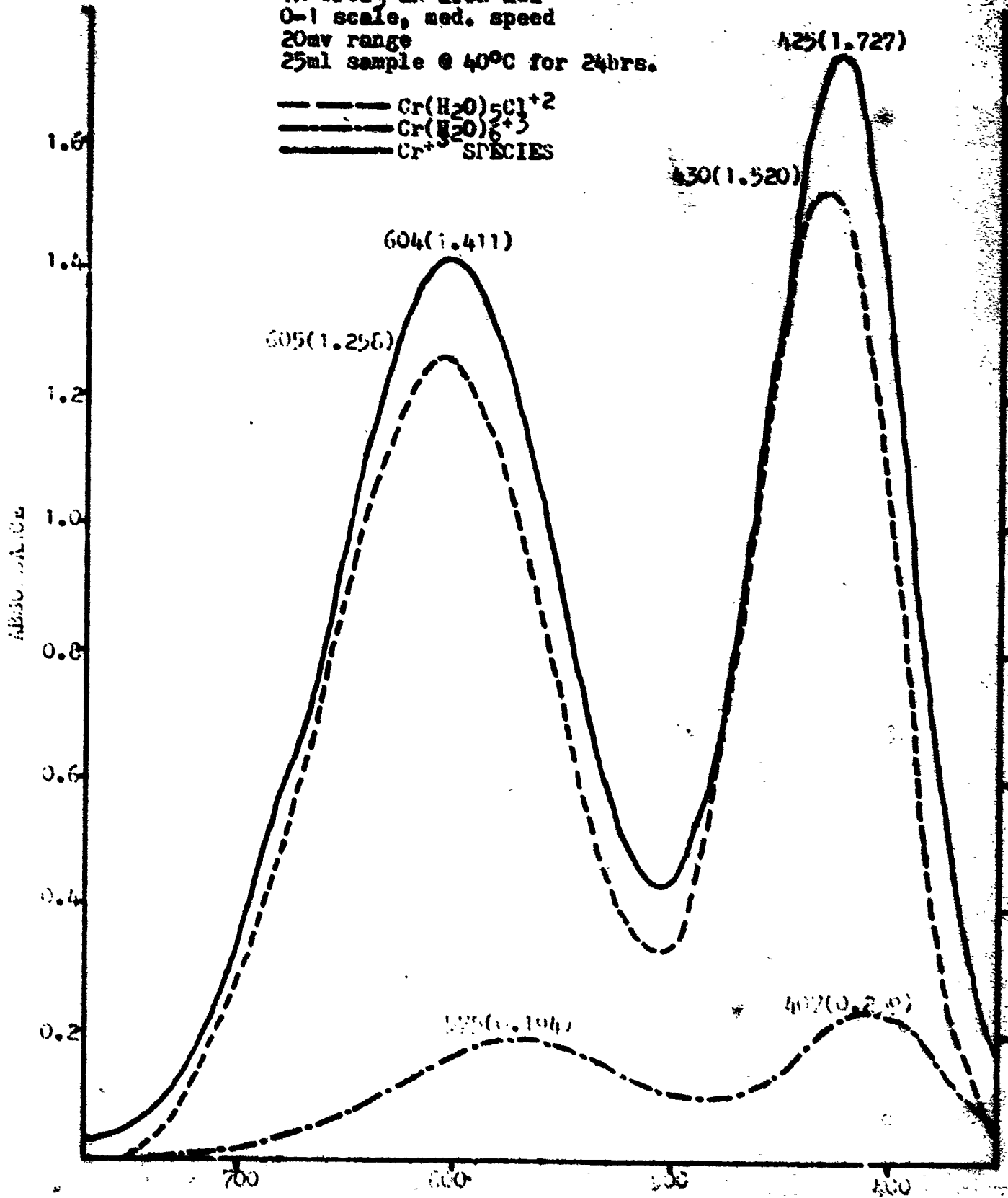
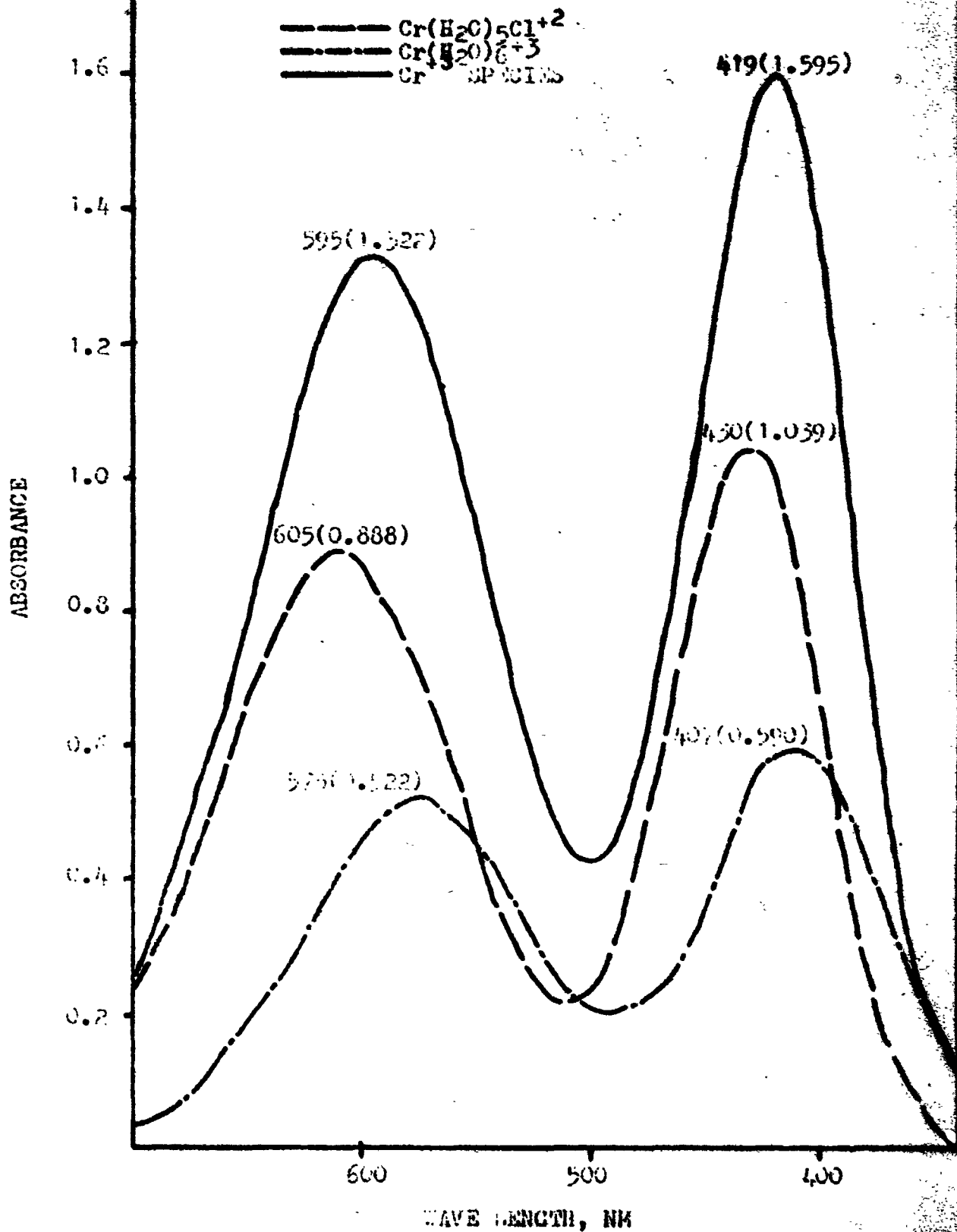


FIGURE 14- SPECTRA #52

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OF POOR QUALITY

1M CrCl₃ in 2.0N HCl
 0-1 scale, med. speed
 20mv range
 10ml sample @ 55°C for 24hrs.



DETERMINATION OF CONCENTRATIONS OF TWO SPECIES
IN SOLUTION USING LASER SPECTROSCOPY

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SPECTRA WERE OBTAINED FROM THE STUDY-RETAINED FILE UNDER NO.

WAVELENGTH	CONCENTRATION	STANDARD DEVIATION	RELATIVE AVERAGE DEVIATION	RELATIVE AVERAGE DEVIATION
652	0.178	11.15	6.27	0.1
656	1.069	18.82	17.59	0.1
658	1.227	15.82	12.89	0.1
656	1.038	6.93	6.69	0.1
637	0.880	15.04	16.84	0.1
642	0.941	13.11	13.95	0.1
642	1.337	18.91	14.16	0.1
616	1.565	19.82	16.52	0.1
388	0.988	7.38	10.18	0.1
378	0.495	2.55	11.92	0.1

THE CONCENTRATION OF THE FIRST SPECIES IS .2562 MOLAR

THE CONCENTRATION OF THE SECOND SPECIES IS .3537 MOLAR

FIRST SPECIES STANDARD DEVIATION IS 0.115
SECOND SPECIES STANDARD DEVIATION IS 0.105

FIRST SPECIES RELATIVE AVERAGE DEVIATION IS 15.22%
SECOND SPECIES RELATIVE AVERAGE DEVIATION IS 21.79%

DATA

CONCENTRATION (M)	CONCENTRATION (M)
.113775	.119875
.120775	.126875
.126875	.133875
.134575	.141875
.140775	.149875
.148775	.157875
.156775	.165875
.164775	.173875
.172775	.181875
.180775	.189875
.188775	.197875
.196775	.205875
.204775	.213875
.212775	.221875
.220775	.229875
.228775	.237875
.236775	.245875
.244775	.253875
.252775	.261875
.260775	.269875
.268775	.277875
.276775	.285875
.284775	.293875
.292775	.301875
.300775	.309875
.308775	.317875
.316775	.325875
.324775	.333875
.332775	.341875
.340775	.349875
.348775	.357875
.356775	.365875
.364775	.373875
.372775	.381875
.380775	.389875
.388775	.397875
.396775	.405875
.404775	.413875
.412775	.421875
.420775	.429875
.428775	.437875
.436775	.445875
.444775	.453875
.452775	.461875
.460775	.469875
.468775	.477875
.476775	.485875
.484775	.493875
.492775	.501875
.500775	.509875
.508775	.517875
.516775	.525875
.524775	.533875
.532775	.541875
.540775	.549875
.548775	.557875
.556775	.565875
.564775	.573875
.572775	.581875
.580775	.589875
.588775	.597875
.596775	.605875
.604775	.613875
.612775	.621875
.620775	.629875
.628775	.637875
.636775	.645875
.644775	.653875
.652775	.661875
.660775	.669875
.668775	.677875
.676775	.685875
.684775	.693875
.692775	.701875
.700775	.709875
.708775	.717875
.716775	.725875
.724775	.733875
.732775	.741875
.740775	.749875
.748775	.757875
.756775	.765875
.764775	.773875
.772775	.781875
.780775	.789875
.788775	.797875
.796775	.805875
.804775	.813875
.812775	.821875
.820775	.829875
.828775	.837875
.836775	.845875
.844775	.853875
.852775	.861875
.860775	.869875
.868775	.877875
.876775	.885875
.884775	.893875
.892775	.901875
.900775	.909875
.908775	.917875
.916775	.925875
.924775	.933875
.932775	.941875
.940775	.949875
.948775	.957875
.956775	.965875
.964775	.973875
.972775	.981875
.980775	.989875
.988775	.997875
.996775	1.005875
1.004775	1.013875
1.012775	1.021875
1.020775	1.029875
1.028775	1.037875
1.036775	1.045875
1.044775	1.053875
1.052775	1.061875
1.060775	1.069875
1.068775	1.077875
1.076775	1.085875
1.084775	1.093875
1.092775	1.101875
1.100775	1.109875
1.108775	1.117875
1.116775	1.125875
1.124775	1.133875
1.132775	1.141875
1.140775	1.149875
1.148775	1.157875
1.156775	1.165875
1.164775	1.173875
1.172775	1.181875
1.180775	1.189875
1.188775	1.197875
1.196775	1.205875
1.204775	1.213875
1.212775	1.221875
1.220775	1.229875
1.228775	1.237875
1.236775	1.245875
1.244775	1.253875
1.252775	1.261875
1.260775	1.269875
1.268775	1.277875
1.276775	1.285875
1.284775	1.293875
1.292775	1.301875
1.300775	1.309875
1.308775	1.317875
1.316775	1.325875
1.324775	1.333875
1.332775	1.341875
1.340775	1.349875
1.348775	1.357875
1.356775	1.365875
1.364775	1.373875
1.372775	1.381875
1.380775	1.389875
1.388775	1.397875
1.396775	1.405875
1.404775	1.413875
1.412775	1.421875
1.420775	1.429875
1.428775	1.437875
1.436775	1.445875
1.444775	1.453875
1.452775	1.461875
1.460775	1.469875
1.468775	1.477875
1.476775	1.485875
1.484775	1.493875
1.492775	1.501875
1.500775	1.509875
1.508775	1.517875
1.516775	1.525875
1.524775	1.533875
1.532775	1.541875
1.540775	1.549875
1.548775	1.557875
1.556775	1.565875
1.564775	1.573875
1.572775	1.581875
1.580775	1.589875
1.588775	1.597875
1.596775	1.605875
1.604775	1.613875
1.612775	1.621875
1.620775	1.629875
1.628775	1.637875
1.636775	1.645875
1.644775	1.653875
1.652775	1.661875
1.660775	1.669875
1.668775	1.677875
1.676775	1.685875
1.684775	1.693875
1.692775	1.701875
1.700775	1.709875
1.708775	1.717875
1.716775	1.725875
1.724775	1.733875
1.732775	1.741875
1.740775	1.749875
1.748775	1.757875
1.756775	1.765875
1.764775	1.773875
1.772775	1.781875
1.780775	1.789875
1.788775	1.797875
1.796775	1.805875
1.804775	1.813875
1.812775	1.821875
1.820775	1.829875
1.828775	1.837875
1.836775	1.845875
1.844775	1.853875
1.852775	1.861875
1.860775	1.869875
1.868775	1.877875
1.876775	1.885875
1.884775	1.893875
1.892775	1.901875
1.900775	1.909875
1.908775	1.917875
1.916775	1.925875
1.924775	1.933875
1.932775	1.941875
1.940775	1.949875
1.948775	1.957875
1.956775	1.965875
1.964775	1.973875
1.972775	1.981875
1.980775	1.989875
1.988775	1.997875
1.996775	2.005875
2.004775	2.013875
2.012775	2.021875
2.020775	2.029875
2.028775	2.037875
2.036775	2.045875
2.044775	2.053875
2.052775	2.061875
2.060775	2.069875
2.068775	2.077875
2.076775	2.085875
2.084775	2.093875
2.092775	2.101875
2.100775	2.109875
2.108775	2.117875
2.116775	2.125875
2.124775	2.133875
2.132775	2.141875
2.140775	2.149875
2.148775	2.157875
2.156775	2.165875
2.164775	2.173875
2.172775	2.181875
2.180775	2.189875
2.188775	2.197875
2.196775	2.205875
2.204775	2.213875
2.212775	2.221875
2.220775	2.229875
2.228775	2.237875
2.236775	2.245875
2.244775	2.253875
2.252775	2.261875
2.260775	2.269875
2.268775	2.277875
2.276775	2.285875
2.284775	2.293875
2.292775	2.301875
2.300775	2.309875
2.308775	2.317875
2.316775	2.325875
2.324775	2.333875
2.332775	2.341875
2.340775	2.349875
2.348775	2.357875
2.356775	2.365875
2.364775	2.373875
2.372775	2.381875
2.380775	2.389875
2.388775	2.397875
2.396775	2.405875
2.404775	2.413875
2.412775	2.421875
2.420775	2.429875
2.428775	2.437875
2.436775	2.445875
2.444775	2.453875
2.452775	2.461875
2.460775	2.469875
2.468775	2.477875
2.476775	2.485875
2.484775	2.493875
2.492775	2.501875
2.500775	2.509875
2.508775	2.517875
2.516775	2.525875
2.524775	2.533875
2.532775	2.541875
2.540775	2.549875
2.548775	2.557875
2.556775	2.565875
2.564775	2.573875
2.572775	2.581875
2.580775	2.589875
2.588775	2.597875
2.596775	2.605875
2.604775	2.613875
2.612775	2.621875
2.620775	2.629875
2.628775	2.637875
2.636775	2.645875
2.644775	2.653875
2.652775	2.661875
2.660775	2.669875
2.668775	2.677875
2.676775	2.685875
2.684775	2.693875
2.692775	2.701875
2.700775	2.709875
2.708775	2.717875
2.716775	2.725875
2.724775	2.733875
2.732775	2.741875
2.740775	2.749875
2.748775	2.757875
2.756775	2.765875
2.764775	2.773875
2.772775	2.781875
2.780775	2.789875
2.788775	2.797875
2.796775	2.805875
2.804775	2.813875
2.812775	2.821875
2.820775	2.829875
2.828775	2.837875
2.836775	2.845875
2.844775	2.853875
2.852775	2.861875
2.860775	2.869875
2.868775	2.877875
2.876775	2.885875
2.884775	2.893875
2.892775	2.901875
2.900775	2.909875
2.908775	2.917875
2.916775	2.925875
2.924775	2.933875
2.932775	2.941875
2.940775	2.949875
2.948775	2.957875
2.956775	2.965875
2.964775	2.973875
2.972775	2.981875
2.980775	2.989875
2.988775	2.997875
2.996775	3.005875
3.004775	3.013875
3.012775	3.021875
3.020775	3.029875
3.028775	3.037875
3.036775	3.045875
3.044775	3.053875
3.052775	3.061875
3.060775	3.069875
3.068775	3.077875
3.076775	3.085875
3.084775	3.093875
3.092775	3.101875
3.100775	3.109875
3.108775	3.117875
3.116775	

SPECTRAL RELATIONSHIP BETWEEN THE FIRST AND SECOND SPECIES

WAVELENGTH (nm)	RELATIVE INTENSITY (%)	RELATIVE INTENSITY (%)	RELATIVE INTENSITY (%)	RELATIVE INTENSITY (%)
280	0.000	10.00	10.00	0.00
285	0.000	10.00	10.00	0.00
290	0.000	10.00	10.00	0.00
295	0.000	10.00	10.00	0.00
300	0.000	10.00	10.00	0.00
305	0.000	10.00	10.00	0.00
310	0.000	10.00	10.00	0.00
315	0.000	10.00	10.00	0.00
320	0.000	10.00	10.00	0.00
325	0.000	10.00	10.00	0.00
330	0.000	10.00	10.00	0.00
335	0.000	10.00	10.00	0.00
340	0.000	10.00	10.00	0.00
345	0.000	10.00	10.00	0.00
350	0.000	10.00	10.00	0.00
355	0.000	10.00	10.00	0.00
360	0.000	10.00	10.00	0.00
365	0.000	10.00	10.00	0.00
370	0.000	10.00	10.00	0.00

THE CONCENTRATION OF THE FIRST SPECIES IS 0.007 MOLAR
 THE CONCENTRATION OF THE SECOND SPECIES IS 0.045 MOLAR

FIRST SPECIES STANDARD DEVIATION IS 0.035
 SECOND SPECIES STANDARD DEVIATION IS 0.035

FIRST SPECIES RELATIVE AVERAGE DEVIATION IS 5.16%
 SECOND SPECIES RELATIVE AVERAGE DEVIATION IS 11.0%

DATA
 WAVELENGTH (nm) CONCENTRATION (MOLAR)

280	0.000	10.00
285	0.000	10.00
290	0.000	10.00
295	0.000	10.00
300	0.000	10.00
305	0.000	10.00
310	0.000	10.00
315	0.000	10.00
320	0.000	10.00
325	0.000	10.00
330	0.000	10.00
335	0.000	10.00
340	0.000	10.00
345	0.000	10.00
350	0.000	10.00
355	0.000	10.00
360	0.000	10.00
365	0.000	10.00
370	0.000	10.00
375	0.000	10.00
380	0.000	10.00
385	0.000	10.00
390	0.000	10.00
395	0.000	10.00
400	0.000	10.00
405	0.000	10.00
410	0.000	10.00
415	0.000	10.00
420	0.000	10.00
425	0.000	10.00
430	0.000	10.00
435	0.000	10.00
440	0.000	10.00
445	0.000	10.00
450	0.000	10.00
455	0.000	10.00
460	0.000	10.00
465	0.000	10.00
470	0.000	10.00
475	0.000	10.00
480	0.000	10.00
485	0.000	10.00
490	0.000	10.00
495	0.000	10.00
500	0.000	10.00
505	0.000	10.00
510	0.000	10.00
515	0.000	10.00
520	0.000	10.00
525	0.000	10.00
530	0.000	10.00
535	0.000	10.00
540	0.000	10.00
545	0.000	10.00
550	0.000	10.00
555	0.000	10.00
560	0.000	10.00
565	0.000	10.00
570	0.000	10.00
575	0.000	10.00
580	0.000	10.00
585	0.000	10.00
590	0.000	10.00
595	0.000	10.00
600	0.000	10.00
605	0.000	10.00
610	0.000	10.00
615	0.000	10.00
620	0.000	10.00
625	0.000	10.00
630	0.000	10.00
635	0.000	10.00
640	0.000	10.00
645	0.000	10.00
650	0.000	10.00
655	0.000	10.00
660	0.000	10.00
665	0.000	10.00
670	0.000	10.00
675	0.000	10.00
680	0.000	10.00
685	0.000	10.00
690	0.000	10.00
695	0.000	10.00
700	0.000	10.00
705	0.000	10.00
710	0.000	10.00
715	0.000	10.00
720	0.000	10.00
725	0.000	10.00
730	0.000	10.00
735	0.000	10.00
740	0.000	10.00
745	0.000	10.00
750	0.000	10.00
755	0.000	10.00
760	0.000	10.00
765	0.000	10.00
770	0.000	10.00
775	0.000	10.00
780	0.000	10.00
785	0.000	10.00
790	0.000	10.00
795	0.000	10.00
800	0.000	10.00
805	0.000	10.00
810	0.000	10.00
815	0.000	10.00
820	0.000	10.00
825	0.000	10.00
830	0.000	10.00
835	0.000	10.00
840	0.000	10.00
845	0.000	10.00
850	0.000	10.00
855	0.000	10.00
860	0.000	10.00
865	0.000	10.00
870	0.000	10.00
875	0.000	10.00
880	0.000	10.00
885	0.000	10.00
890	0.000	10.00
895	0.000	10.00
900	0.000	10.00
905	0.000	10.00
910	0.000	10.00
915	0.000	10.00
920	0.000	10.00
925	0.000	10.00
930	0.000	10.00
935	0.000	10.00
940	0.000	10.00
945	0.000	10.00
950	0.000	10.00
955	0.000	10.00
960	0.000	10.00
965	0.000	10.00
970	0.000	10.00
975	0.000	10.00
980	0.000	10.00
985	0.000	10.00
990	0.000	10.00
995	0.000	10.00
1000	0.000	10.00

THE CONCENTRATION OF THE FIRST SPECIES IS 0.007 MOLAR
 THE CONCENTRATION OF THE SECOND SPECIES IS 0.045 MOLAR
 FIRST SPECIES STANDARD DEVIATION IS 0.035
 SECOND SPECIES STANDARD DEVIATION IS 0.035
 FIRST SPECIES RELATIVE AVERAGE DEVIATION IS 5.16%
 SECOND SPECIES RELATIVE AVERAGE DEVIATION IS 11.0%

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