



REFERENCES

1. Knevel, A.M., and DiGangi, F.E., Jenkin's Quantitative Pharmaceutical Chemistry, pp 115-129, McGraw-Hill Book Company, New York, 7th ed., 1977.
2. Skoog, D.A., and West, D.M., Foundations of Analytical Chemistry, pp 262-274, CBS College Publishing, Japan, 4th ed., 1982.
3. Kolthoff, I.M., and Scandal, E.B., Textbook of Quantitative Inorganic Analyses, pp 483-489, MacMillan, New York, 1949.
4. Kolthoff, I.M., and Stenger, V.A., Volumetric Analysis I, pp 260-264, Interscience Publishers Inc., New York, 2nd ed., 1942.
5. Anfalt, T., and Jagner, D., "The Precision and Accuracy of Some Current Methods for Potentiometric End-Point Determination with Reference to a Computer-Calculated Titration Curve," Anal. Chim. Acta, 57, 165-176, 1971.
6. Tubbs, C.F., "Determination of Potentiometric Titration Inflection Point by the Concentric Arcs Method," Anal. Chem., 26, 1670-1671, 1954.
7. Vogel, A.I., A Textbook of Quantitative Inorganic Analysis, pp 596-600, Longman Group Limited, London, 4th ed., 1978.
8. Cohen, S.R., "A Simple Graphical Method for Locating the End Point of a pH or a Potentiometric Titration," Anal. Chem., 38, 158, 1966.

9. Fotuin, J.M.H., " Method for Determination of the Equivalence Point in Potentiometric Titrations," Anal. Chim. Acta., 24, 175-191, 1961.
10. Gran, G., " Determination of the Equivalence Point in Potentiometric Titrations," Acta Chem. Scand., 4, 559-577, 1950.
11. Johansson, A., and Gran, G., " Extension of the Gran I Method for Calculation of the Equivalence Volume in Acid-Base Titrations," Analyst, 106, 802-810, 1980.
12. Gran, G., and Johansson, A., " Further Extension of the Gran I Method for Calculation of the Equivalence Volume in Acid-Base Titrations," Analyst, 106, 231-242, 1981.
13. Liteanu, C., and Cormos, D., " Contribution au Probleme de la Determination du Point D'Equivalence-I," Talanta, 7, 18-24, 1960.
14. Cavanagh, B., " A General (Exact) Equation to the Potentiometric-titration Curve," J. Chem. Soc., 1425-1447, 1930.
15. Herringshaw, J.F., " A Rapid Method of Forecasting the End-point in Potentiometric Titrations," Analyst, 87, 463-466, 1962.
16. Barry, D.M., and Meites, L., " Titrimetric Applications of Multiparametric Curve-Fitting Part 1. Potentiometric Titrations of Weak Bases with Strong Acids at Extreme Dilutions," Anal. Chim. Acta, 68, 435-445, 1974.

17. Johansson, A., " Automatic Titration by Stepwise Addition of Equal Volumes of Titrant. Part I," Analyst, 95, 535-540, 1970.
18. Gran, G., " Determination of the Equivalence Point in Potentiometric Titrations. Part II," Analyst, 77, 661-670, 1952.
19. Rossatti, F.J.C., and Rossatti, H., " Potentiometric Titrations Using Gran Plots," J. Chem. Ed., 42, 375-378, 1965.
20. Christian, G.D., Analytical Chemistry, pp 323-324, John Wiley & Sons, New York, 3rd ed., 1980.
21. Skoog, D.A., and West, D.M., Principles of Instrumental Analysis, pp 562-563, Holt-Saunders Japan Ltd., 2nd ed., 1981.
22. Westcott, C.C., " Ion Selective Measurements by Gran Plots with a Gran Ruler," Anal. Chim. Acta, 86, 269-271, 1976.
23. Johansson, A., and Johansson, S., " Automatic Titration by Stepwise Addition of Equal Volumes of Titrant. Part III," Analyst, 103, 305-316, 1978.
24. Johansson, A., and Johansson, S., " Automatic Titration by Stepwise Addition of Equal Volumes of Titrant. Part IV," Analyst, 104, 601-612, 1979.
25. Benet, L.Z., and Goyan, J.E., " Determination of the Stability Constants of Tetracycline Complexes," J. Pharm. Sci., 54, 983-987, 1965.

26. Benet, L.Z., and Goyan, J.E., " Nonlogarithmic Titration Curves for the Determination of Dissociation Constants and Purity," J. Pharm. Sci., 54, 1179-1182, 1965.
27. Benet, L.Z., and Goyan, J.E., " Potentiometric Determination of Dissociation Constants," J. Pharm. Sci., 56, 665-680, 1967.
28. Frazer, J.W., Krey, A.M., Selig, W., and Lim, R., " Interactive Experimentation Employing Ion-Selective Electrodes," Anal. Chem., 47, 869-875, 1975.
29. Ingman, F., and Still, E., " Graphic Method for the Determination of Titration End-Points," Talanta, 13, 1431-1442, 1966.
30. McCallum, C., and Midgley, D., " Improved Linear Titration Plots for Potentiometric Precipitation and Strong Acid - Strong Base Titrations," Anal. Chim. Acta, 65, 155-162, 1973.
31. Setnikar, I., " Ionization of Basea with Limited Solubility ," J. Pharm. Sci., 55, 1190-1195, 1966.
32. Levy, R., and Rowland, M., " Dissociation Constants of Sparingly Soluble Substance : Nonlogarithmic Linear Titration Curves," J. Pharm. Sci., 60, 1155-1159, 1971.
33. The United States Pharmacopeia, 21st rev. The National Formulary, 16th ed., pp 1098, United States Pharmacopeial Convention Inc., Rockville, Md., 1985.

34. Ibid, pp 299.
35. Ibid, pp 929-930.
36. Ibid, pp 340.
37. Ibid, pp 829-830.
38. Ibid, pp 202.
39. Ibid, pp 913.
40. Doerge, R.F., ed., Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, pp 841-847, J.P. Lippincott Company, Philadelphia, 8th ed., 1982.
41. Gran's Plots and Other Schemes, Newsletter of Orion Research Incorporated, 2, 11, 1970.
42. Hargreaves, M.K., and Richardson, P.J., " The Titration and the Apparent Dissociation Constants of Weak Acids in Mixed Aqueous Solvents," J. Chem. Soc., 3111-3116, 1958
43. Cavill, G.W.K., Gibson, N.A., and Nyholm, R.S., " The Dissociation Constants of Some p-Alkoxybenzoic Acids," J. Chem. Soc., 2466-2470, 1949.
44. Gutbezahl, B., and Grunwald, E., " The Acidity and Basicity Scale in the System Ethanol-Water. The Evaluation of Degenerate Acidity Coefficients for Single Ions," J. Amer. Chem. Soc., 75, 565-574, 1953.
45. Bates, R.G., Paabo, M., and Robinson, R.A., " Interpretation of pH Measurements in Alcohol-Water Solvents," J. Phys. Chem., 67, 1833-1838, 1963.



APPENDIX

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Program I

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10 REM GRAN'S PLOT
20 CLS:PRINT "PUT PA'ER ON PRINTER"
30 DIM V(40),PH(40),G(40),GH(40)
40 INPUT "Enter file name ";C$
60 OPEN "i",1,C$
70 INPUT#1,D$,PKW,VO,N
80 X=1
90 INPUT#1,V,PH
100 V(X)=V : PH(X)=PH
110 IF EOF(1) THEN 130
120 X=X+1:GOTO 90
130 LPRINT"Compound name is ";D$;:LPRINT TAB(40;"No. of data point = ";X
140 LPRINT "pKw = ";PKW;:LPRINT TAB(15)"Initial volumn = ";VO;
150 LPRINT TAB(40) "Normality of titrant =";N
160 FOR I =1 TO X
170 OH = 10^(PH(I)-PKW)
180 H=10^-PH(I)
190 G(I) = V(I)*N*(H-OH)*(VO+V(I))
200 GH(I) = H*G(I)
210 NEXT I
220 LPRINT C$:LPRINT
230 LPRINT TAB(3) "Vol"; : LPRINT TAB(12) "pH";
240 LPRINT TAB(30) "G(I)"; : LPRINT TAB(48) "GH(I)"
250 FOR I = 1 TO X
260 LPRINT TAB(2) USING "#.##";V(I); : LPRINT TAB(11) USING "#.##";PH(I);
270 LPRINT TAB(26) USING "+#.#####^";G(I);
280 LPRINT TAB(44) USING "+#.#####^";GH(I)
290 NEXT I
300 LPRINT:LPRINT
310 CLS:LPRINT"LINEAR CORRELATION COEFFICIENT AND REGRESSION"
320 PRINT:PRINT
330 DIM X(X),Y(X)
340 FOR I=1 TO X
350 X(I)=G(I):Y(I)=GH(I)
360 NEXT I
370 REM* FIND XSUM,YSUM,XYSUM,X2SUM,Y2SUM
380 INPUT "HOW MANY TERM YOU WANT TO SOURCE ";P
390 LPRINT "No. OF USED DATA";P
400 LPRINT
410 LPRINT "Exper.";
420 LPRINT TAB(13) "Correlation";:LPRINT TAB(30) "Slope";
430 LPRINT TAB(43) "Y intercept";:LPRINT TAB(60) "X intercept"
440 LPRINT
450 FOR J=0 TO X-P
460 XBAR=0 : YBAR=0 : XYSUM=0 : NUM=0 : DEN=0
470 XSUM=0 : YSUM=0 : X2SUM=0 : Y2SUM=0
480 FOR K=1 TO P
490 I=J+K
500 XSUM=XSUM+X(I)
510 YSUM=YSUM+Y(I)
520 U=X(I)*Y(I) : XYSUM=XYSUM+U
530 U=X(I)*X(I) : X2SUM=X2SUM+U
540 U=Y(I)*Y(I) : Y2SUM=Y2SUM+U
550 NEXT K
560 XBAR=XSUM/P : YBAR=YSUM/P
570 CLS
580 REM*CALCULATE NUMERATOR
590 NUM=XYSUM-((XSUM*YSUM)/P)
600 REM*CALCULATE DENOMINATOR
610 DEN=(SQR(X2SUM-((XSUM^2)/P)))*(SQR(Y2SUM-((YSUM^2)/P)))
620 REM*CALCULATE CORRERATION
630 R=NUM/DEN
640 REM*CALCULATE SLOPE OF REGRESSION LINE
650 B=(YSUM-((XSUM*YSUM)/P))/(X2SUM-(XSUM^2/P))
660 REM*CALCULATE Y INTERCEPT
670 A=YBAR-(B*XBAR)
680 REM*CALCULATE X INTERCEPT
690 AX=-A/B
700 LPRINT J+1;"-";J;P;
710 LPRINT TAB(11) USING "+.#####";R;: LPRINT TAB(27) USING "+.#####^";B;
720 LPRINT TAB(42) USING "+.#####^";A;
730 LPRINT TAB(59) USING "+.#####^";AX
740 NEXT J
750 LPRINT : LPRINT "*****" :LPRINT
760 INPUT "Enter 1 for more range OR 2 to quit ";C
770 IF C=2 THEN END
780 GOTO 380

```


Program II

```

1 *****
2 *
3 *                               DATA
4 *
5 *****
10 INPUT "Enter file name ";C$
20 INPUT "Enter compound name ";D$
30 INPUT "pKw ";PKW
40 INPUT "Initial volumn ";VO
50 INPUT "Normality of titrant ";N
60 INPUT "No. of data point ";X
70 DIM V(X), PH(X)
80 FOR I=1 TO X
90 PRINT "Volumn (";I;" ) = ";
100 INPUT V(I)
110 NEXT I
120 INPUT "Enter 1 for all volumn is true OR 2 to correct ";D
130 IF D=1 GOTO 180
140 INPUT "What No. ";E
150 PRINT "Volumn (";E;" ) = ";
160 INPUT V(E)
170 GOTO 120
180 FOR I=1 TO X
190 PRINT "pH (";I;" ) = ";
200 INPUT PH(I)
210 NEXT I
220 INPUT "Enter 1 for all pH is true OR 2 to correct ";D
230 IF D=1 GOTO 280
240 INPUT "What No. ";E
250 PRINT "pH (";E;" ) = ";
260 INPUT PH(E)
270 GOTO 220
280 OPEN "O",1,C$
290 PRINT#1,D$
300 PRINT#1,PKW
310 PRINT#1,VO
320 PRINT#1,N
330 FOR I=1 TO X
340 V=V(I) : PH=PH(I)
350 PRINT#1,V,PH
360 NEXT I
370 CLOSE 1
380 CLS: PRINT : PRINT : PRINT : PRINT TAB(37) "THE END"
390 *****

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Note :

a. Program I was employed for execution the end point volumes of a Gran function which accounted for autoprotolysis of water. The program was also utilized for other Gran function by changing arithmetic functions in line number 170 - 200 with respect to those Gran functions.

b. Program II was exploited for collecting data which would be input in program I for calculations.

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