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DESIGN CONSIDERATIONS OF REACTOR CONTAINMENT SPRAY SYSTEMS – PART IV. CALCULATION OF IODINE-WATER PARTITION COEFFICIENTS

L. F. Parsly

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DESIGN CONSIDERATIONS OF REACTOR CONTAINMENT SPRAY SYSTEMS – PART IV. CALCULATION OF IODINE-WATER PARTITION COEFFICIENTS

L. F. Parsly

JANUARY 1970

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee
operated by
UNION CARBIDE CORPORATION
for the
U. S. ATOMIC ENERGY COMMISSION

FOREWORD

The Spray and Absorption Technology Program is coordinated by Oak Ridge National Laboratory for the AEC. The program involves research on all aspects of containment spray systems proposed for use as an engineered safety feature in pressurized water reactor containment buildings and investigations of certain aspects of the pool-pressure-suppression containment concept as applied to boiling water reactors.

This report provides a detailed discussion of the iodine-water partition coefficient and gives the numerical value of the coefficient over a wide spectrum of temperature, pH, and concentration conditions.

This is the fourth report in a series designed to present program information pertinent to actual plant design considerations. Additional reports in this series include:

T. H. Row, L. F. Parsly, and H. E. Zittel, *Design Considerations of Reactor Containment Spray Systems – Part I,* USAEC Report ORNL-TM-2412, April 1969.

C. Stuart Patterson and William T. Humphries, *Design Considerations of Reactor Containment Spray Systems – Part II. Removal of Iodine and Methyl Iodide from Air by Liquid Solutions,* USAEC Report ORNL-TM-2412, Part II, August 1969.

J. C. Griess and A. L. Bacarella, *Design Considerations of Reactor Containment Spray Systems – Part III. The Corrosion of Materials in Spray Solutions,* USAEC Report ORNL-TM-2412, Part III.

Thomas H. Row
Technical Coordinator
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DESIGN CONSIDERATIONS OF REACTOR CONTAINMENT SPRAY SYSTEMS – PART IV. CALCULATION OF IODINE-WATER PARTITION COEFFICIENTS

L. F. Parsly

ABSTRACT

Procedures for calculating the partition coefficient of iodine between water and air from solubility, vapor pressure, and hydrolysis equilibrium data are described. Results are presented in tabular form covering the pH range 5.0 to 9.5, the temperature range 25 to 150°C, and dissolved iodine concentrations ranging from saturated solutions down to 10^{-9} mole/liter.

INTRODUCTION

Approximately two years ago a spray and pool absorption technology program was started at the Oak Ridge National Laboratory. The purpose of the program was to generate and disseminate information regarding the performance of such engineered safety systems as containment spray systems and pressure suppression pools. A document describing the scope and purpose of the program has recently been issued.[1] Briefly, the program comprises a search for more effective solution reagents than those now in use, radiation stability and corrosion studies of solutions which it is proposed to use, wind tunnel and pilot-plant studies of fission product absorption by drops and sprays, and pilot-plant studies of condensation of steam and absorption of fission products by suppression pools.

The series of reports entitled "Design Considerations of Reactor Containment Spray Systems" was started to disseminate information which would be of value to reactor designers and safety reviewers concerned with containment spray systems. Part I of the series[2] covers reagent requirements for a design basis accident, the question of gas and liquid film resistance, drop saturation effects, drop size effects, scale-up problems, radiolytic H_2 generation, radiolytic solids generation, loss of solution reactivity due to radiolytic and thermal degradation, and radiolytic pH change. Part II of the series covers solution search work done as part of the program.[3]

An important quantity in the evaluation of containment spray systems is the partition coefficient (H). We define H as the ratio of concentration in the gas phase to concentration in the liquid phase at equilibrium. Because iodine undergoes a complicated series of hydrolysis reactions, H is a complicated function of temperature, pH, and concentration. A procedure for calculating H was suggested by Eggleton[4] and forms the basis of this report.

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[1] T. H. Row, *Spray and Pool Absorption Technology Program,* USAEC Report ORNL-4360.

[2] T. H. Row, L. F. Parsly, and H. E. Zittel, *Design Considerations of Reactor Containment Spray Systems,* USAEC Report ORNL-TM-2412, Oak Ridge National Laboratory (April 1969).

[3] C. S. Patterson and W. T. Humphries, *Removal of Iodine and Methyl Iodide from Air by Liquid Solutions,* USAEC Report ORNL-TM-2412, Part II (in press).

[4] A. E. J. Eggleton, *A Theoretical Examination of Iodine-Water Partition Coefficients,* AERE-R-4887 (February 1967).

We programmed Eggleton's calculation for a digital computer and have executed the calculation over the range of temperature, pH, and concentration likely to be of interest in the water reactor safety program. The purpose of this report is to make the results available to those who wish to use them, to illustrate what happens when certain of the assumptions are changed, and to discuss the chemical basis and the data sources used for the benefit of those who may wish to make an evaluation of the basis used for the calculations.

CHEMISTRY OF IODINE IN AQUEOUS SOLUTIONS

The chemistry of iodine in aqueous solutions has been studied extensively during the past century. Iodine can exist in the following oxidation states:

-1 I^-

0 I_2

$+1$ I^+, H_2OI^+

$+5$ IO_3^-

$+7$ IO_4^-

Eggleton[4] lists the following reactions and equilibria:

1. $I_2(g) \rightleftharpoons I_2(aq)$ $\qquad K_1 = \dfrac{[I_2]_{aq}}{[I_2]_g}$

2. $I_2(aq) + I^- \rightleftharpoons I_3^-$ $\qquad K_2 = \dfrac{[I_3^-]}{[I_2]_{aq}[I^-]}$

3. $I_2(aq) + H_2O \rightleftharpoons H^+ + I^- + HIO$ $\qquad K_3 = \dfrac{[H^+]\ [I^-]\ [HIO]}{[I_2]_{aq}}$

4. $I_2(aq) + H_2O \rightleftharpoons H_2OI^+ + I^-$ $\qquad K_4 = \dfrac{[H_2OI^+]\ [I^-]}{[I_2]_{aq}}$

5. $3I_2(aq) + 3H_2O \rightleftharpoons IO_3^- + 5I^- + 6H^+$ $\qquad K_5 = \dfrac{[IO_3^-]\ [I^-]^5\ [H^+]^6}{[I_2]_{aq}^3}$

6. $HIO \rightleftharpoons H^+ + IO^-$ $\qquad K_6 = \dfrac{[H^+]\ [IO^-]}{[HIO]}$

7. $IO^- + I^- \rightleftharpoons I_2OH^- + OH^-$ $\qquad K_7 = \dfrac{[I_2OH^-]\ [OH^-]}{[IO^-]\ [I^-]}$

8. $IO^- + I^- \rightleftharpoons I_2O^{2-}$ $\qquad K_8 = \dfrac{[I_2O^{2-}]}{[IO^-]\,[I^-]}$

9. $HIO(g) \rightleftharpoons HIO(aq)$ $\qquad K_9 = \dfrac{[HIO]_{aq}}{[HIO]_g}$

In Eggleton's discussion of the system he points out that some of these reactions are important only for limited ranges of pH and iodine concentration and that reaction 5 is slow enough so that it often may be neglected. The simplest treatment involves the first four equilibria and the relationship

$$[HIO] + [H_2OI^+] = [I^-] + [I_3^-] \; . \tag{10}$$

This expresses the fact that in a hydrolysis there can be no net oxidation or reduction.

The system of equations described above may be solved to give concentrations of all other iodine forms as a function of the concentration of the I_2 species in the liquid. The partition coefficient is then defined as the ratio of the sum of all iodine species in the liquid (converted to equivalent I_2) to the concentration of all iodine species in the gas. The latter is presumed to be I_2 only for the case under discussion.

The system of equations to be solved is:

$$[HIO] = \frac{K_3\,[I_2]_{aq}}{[H^+]\,[I^-]} \; , \tag{11}$$

$$[H_2OI^+] = \frac{K_4\,[I_2]_{aq}}{[I^-]} \; , \tag{12}$$

$$[I_3^-] = K_2\,[I_2]_{aq}\,[I^-] \; , \tag{13}$$

$$[I^-] = \left[\frac{K_4\,[I_2]_{aq}}{1 + K_2\,[I_2]_{aq}} + \frac{K_3\,[I_2]_{aq}}{[H^+]\,(1 + K_2\,[I_2]_{aq})} \right]^{1/2} \; , \tag{14}$$

$$[I_2]_{aq(T)} = [I_2]_{aq} + \frac{1}{2}([HIO] + [H_2OI^+] + [I^-] + 3[I_3^-]) \; , \tag{15}$$

$$H = \frac{[I_2]_{aq(T)}}{[I_2]_g} \; . \tag{16}$$

If the several equilibria are known, the above system of equations is explicit, and solutions may be obtained readily.

VALUES OF THE EQUILIBRIUM CONSTANTS

Values of the several equilibrium constants are available in the literature. In general, we have followed the lead of Eggleton[4] and have used the sources cited in his paper. Where it could be done conveniently, we have reduced the data to equations expressing the equilibrium constants as functions of temperature; where not, we have made tables or graphs, and include appropriate values of the constants as part of the input to the computer.

The data sources and equilibrium constants for Eqs. (1) to (4), which are needed to solve Eqs. (11) to (16), are as follows:

Data for the solubility of iodine in water and for its vapor pressure are available in Seidell[5] and in handbooks.[6] From these it is possible to calculate K_1 if we assume the vapor is an ideal gas. Solubility, vapor pressure, and K_1 values are presented in Table 1. Note that I_2 melts at 112.3°C, and there is a discontinuity at this point.

The constant K_2 is calculated from the relationship reported by Davies and Gwynne:[7]

$$\log K_2 = -48.622 + 16.725 \log T + 3018.8/T \ . \tag{17}$$

For computation purposes, this is used in the form:

$$K_2 = \exp\,(-111.98 + 16.725 \ln T + 6952.3/T) \ . \tag{18}$$

The data reported by Allen and Keefer[8] are used to calculate K_3. They reported values of this at 1.6 and 25°C. These were extrapolated using an Arrhenius plot to cover the range up to 150°C. The results are presented in Table 2.

For K_4, Eggleton reported a value of 1.2×10^{-11} at 25°C taken from Bell and Gelles[9] and a value of 3.9×10^{-11} at 100°C calculated by their method. Since these were fairly close together, we used a linear extrapolation:

$$K_4 = 1.2 \times 10^{-11} + 3.6 \times 10^{-13}(t - 25) \ . \tag{19}$$

COMPUTER PROGRAM

A program to evaluate the constants and calculate the partition coefficients has been written in IBM FORTRAN IV, and a listing is given in the appendix.

In the calculation, the starting point is always to assume that the species I_2 in the solution is in equilibrium with the solid (or liquid) element and its vapor at saturation, and that all other hydrolysis equilibria are satisfied for the saturated solution. Thus the concentrations of all species in the solution are calculated. These are then converted to equivalent I_2 and summed to give the column headed "Total I_2 in Liq." We also calculate and tabulate the base 10 logarithm of the total iodine concentration in solution since this is convenient to have for plotting purposes.

After calculating the concentrations of the several species in the saturated solution and the partition coefficient, the concentration of the I_2 species is halved and the calculations are repeated. This procedure is repeated until the total iodine in the solution is less than 1×10^{-9} mole/liter. We feel that this procedure covers the entire range of liquid-phase concentrations likely to be of practical interest.

Tabulated results covering pH values of 5, 7, 8, 9, 9.2, and 9.5 and temperatures of 25, 50, 75, 100, 125, and 150°C are presented in Tables 3–38 inclusive.

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[5] Seidell, *Solubilities of Inorganic and Metal-Organic Compounds,* Van Nostrand, New York, 1940.

[6] R. H. Perry, C. H. Chilton, and S. D. Kirkpatrick (eds.), *Chemical Engineers' Handbook,* 4th ed., McGraw-Hill, New York, 1963.

[7] M. Davies and E. Gwynne, "The Iodine-Iodide Interaction," *J. Am. Chem. Soc.* **74**, 1748–51 (1952).

[8] T. L. Allen and R. M. Keefer, "The Formation of Hypoiodous Acid and Hydrated Iodine Cation by the Hydrolysis of Iodine," *J. Am. Chem. Soc.* 77, 2734 (1955).

[9] R. P. Bell and E. Gelles, "The Halogen Cations in Aqueous Solution," *J. Chem. Soc.* **1951**, 2734–40.

EFFECT OF IODATE REACTION

Formation of iodate by reaction 5 is generally considered to be a relatively slow process. Eggleton[4] presents results indicating that at 25°C, 10% conversion to iodate would take ten years at pH 5, 11 hr at pH 7, and 4 sec at pH 9. We have not found any kinetic data at other temperatures.

Since the reaction becomes relatively fast at the pH levels (9 to 9.5) that are of interest in the spray program, even at room temperature, and would be expected to go much faster at higher temperatures, it has seemed worth while to consider its effect on the partition coefficient. Following Eggleton,[4] we include Eq. (5) and replace Eq. (10) by:

$$[HIO] + [H_2OI^+] + 5[IO_3^-] = [I^-] + [I_3^-] \ . \tag{20}$$

Solving the equations, we get

$$\frac{K_3[I_2]_{aq}}{[H^+][I^-]} + \frac{K_4[I_2]_{aq}}{[I^-]} + \frac{5K_5[I_{aq}]^3}{[I^-]^5[H^+]^6} = [I^-] + K_2[I_2]_{aq}[I^-] \ . \tag{21}$$

Considering $[I_2]_{aq}$ and $[H^+]$ as known and $[I^-]$ as the unknown X, this reduces to:

$$\frac{C_2}{X} + \frac{C_3}{X^5} = C_1 X \ . \tag{22}$$

This can be solved very rapidly by Horner's method (successive approximation), and a modification of the program has been written to handle the iodate reaction.

Eggleton[4] quoted a value for K_5 of 4×10^{-48} at 25°C reported by Lundberg *et al.*,[10] and we later found that Kolthoff and Stenger[11] report values of 3.8×10^{-49} at 18°C and 5.1×10^{-42} at 60°C. These turn out to be consistent when plotted in the form $\log_{10} K_5$ vs t(°C). The equation is:

$$\log_{10} K_5 = -48.42 + 0.17(t - 18) \ . \tag{23}$$

We have run this calculation for several temperatures and pH values. Typical results are shown in Tables 39–42. There are some obvious problems for solutions saturated with I_2 at high temperature and pH since the program calculates impossibly large values of the total iodine concentration (10^6 moles/liter, for example). Obviously, some of the assumptions are not valid in this case.

The calculations show that when iodate formation is taken into account, the partition coefficients are very markedly increased. Since the kinetic data on the iodate reaction are limited to 25°C, there is no sound basis for knowing under what circumstances the iodate reaction can have a significant effect on the interaction of sprays with airborne iodine.

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[10] W. O. Lundberg, C. S. Vestling, and J. E. Ahlberg, "The Electrode Potential of the Iodate-Iodine Electrode at 25°," *J. Am. Chem. Soc.* 59, 264–68 (1937).

[11] I. M. Kolthoff and V. A. Stenger, *Volumetric Analysis,* vol. II, 2d ed., Interscience, New York, 1947.

EFFECT OF HIO FORMATION

Recently, workers at Idaho Nuclear Corporation[12] have suggested that a volatile iodine form which had not previously been identified is hypoiodous acid (HIO). Hypoiodous acid is an extremely weak acid, its dissociation constant being 4.5×10^{-13} g ion/liter at 20°C.[13]

Until very recently, the existence of HIO in the vapor phase had not been demonstrated. Gelles[14] made an educated guess that HIO should have a free energy of vaporization of 2 ± 1 kcal/mole at 25°C on the basis of known values for HI and H_2O. Styrikovich *et al.*[15] inferred that under certain conditions of dilution and pH, all I_2 in solution should be hydrolyzed to H^+, I^-, and HIO and since I^- is not volatile, any volatile iodine should be HIO.

Within the past few months, workers at Idaho Nuclear Corporation have performed experiments which show positively that HIO is volatile.[16] There is still no experimental evidence respecting the magnitude of its vaporization equilibrium constant (K_9). However, one can assume a value for K_9 and examine the effect of HIO volatility on the iodine partition coefficient.

In this case we have the added equilibrium from Eq. (9) to take into account. Also, since some of the HIO formed has evaporated, we must account for this in the oxidation balance and wind up with:

$$[HIO]_l + \frac{V_g}{V_l}[HIO]_g + [H_2OI^+] = [I^-] + [I_3^-] \ . \tag{24}$$

The programming is quite similar to that for the basic program, but we do note the difference that the gas-to-liquid volume ratio now enters into the calculation and must be supplied as data. We present examples of the results in Tables 43 and 44. This shows that as the iodine concentration decreases, the partition coefficient attains a limit which is approximately twice the partition coefficient for HIO between air and water. There is a good deal of evidence that limiting partition coefficients as low as calculated by this process are not observed in experiments.

CONCLUSIONS

We have presented a technique for calculating the partition coefficient of iodine between water and air in aqueous solutions of varying pH and temperature and variations of the technique to account for the effect of (1) iodate formation and (2) the presence of volatile HIO. The computer program output enables one to examine the breakdown among the various species in solution under varying conditions of temperature and pH.

The validity of the results is dependent on the validity of the assumptions made in the calculation. The chemistry of iodine and its water solutions is enormously complex and has been studied very extensively. For instance, Mellor[17] cites 902 references pertaining to iodine and its inorganic forms. Nevertheless, there

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[12] F. O. Cartan, H. R. Beard, F. A. Duce, and J. H. Keller, "Evidence of the Existence of Hypoiodous Acid as a Volatile Iodine Species Produced in Water-Air Mixtures," Tenth Air Cleaning Conference, New York, Aug. 28, 1968.

[13] A. Skrabal, "Zur Frage nach der Dissoziationskonstanten der Unterjodigen Säure" (On the Question of the Dissociation Constant of Hypoiodous Acid), *Ber.* **75B**, 1570–72 (1942).

[14] E. Gelles, "The Dissociation Energies of Some Oxygen-Halogen Bonds," *Trans. Faraday Soc.* **47**, 1158–60 (1951).

[15] M. A. Styrikovich, O. I. Martynova, K. Ya. Katkovskaya, I. Ya. Dubrovskii, and I. M. Smirneva, "Transfer of Iodine from Aqueous Solutions to Saturated Vapor," *At. Energ.* **17**, 45–49 (1964).

[16] J. H. Keller, Idaho Nuclear Corporation, personal communication.

[17] J. W. Mellor, *A Comprehensive Treatise on Inorganic and Theoretical Chemistry*, suppl. 2, part 1, pp. 836–956, Longmans, 1956.

are numerous questions which cannot be answered by reference to published work. These include such questions as what is the rate of the iodate reaction at higher temperatures, whether HIO is volatile and if so what is the correct magnitude of its vaporization equilibrium constant, etc. The results of a good many experiments, including the work of Watson *et al.*[18] and experiments at the Nuclear Safety Pilot Plant[19] and the Containment Systems Experiment,[20] indicate better iodine removal performance than could be predicted by using partition coefficients calculated by the procedures described here.

In view of these results, we believe that use of the results of this calculation will at worst lead to conservative predictions of the performance of containment spray systems. However, a more complete understanding of the factors which influence the distribution of iodine between water and air would be of great value.

NOMENCLATURE

H = partition coefficient; (concentration in liquid)/(concentration in gas)
K_i = equilibrium constant for reaction i defined by equation in text
V = volume
[X] = concentration of chemical species X
T = Kelvin temperature
t = Celsius temperature
C = known quantity in Eq. (22)
X = unknown quantity in Eq. (22)

Subscripts

aq refers to aqueous phase
g refers to gas phase
l refers to liquid phase
T indicates total of all species present

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[18] L. C. Watson, A. R. Bancroft, and C. W. Koelke, *Iodine Containment by Dousing in NPD-II,* CRCE-979 (1960).

[19] L. F. Parsly and J. K. Franzreb, "Spray Tests in the Nuclear Safety Pilot Plant," pp. 221–31 in *Nuclear Safety Program Annual Progress Report for Period Ending Dec. 31, 1967,* USAEC Report ORNL-4228 (April 1968) (see particularly, run 27).

[20] L. F. Coleman, R. K. Hilliard, C. E. Linderoth, J. D. McCormack, and A. K. Postma, "Large Scale Fission Product Transport Experiments," pp. 2.1–2.23 in *Nuclear Safety Quarterly Report November, December 1968, January 1969,* USAEC Report BNWL-1009, Battelle Memorial Institute, Pacific Northwest Laboratory (March 1969).

APPENDIX

This appendix contains listings of the three computer programs used to generate the tables.

The basic program calculates constants K_2 and K_4 and solves Eqs. (1) to (4) and (10). It is written in FORTRAN IV for the IBM system 360. The variable names are mnemonics; for example, AK1 is K_1, CIMIN is the concentration of I minus. The mathematics are straightforward.

```
C CALCULATION OF PARTITION COEFFICIENT OF IODINE BETWEEN WATER AND AIR
      DO 1 I = 1,100
      READ(50,2,END=3) TEMPC,PH,AK1,AK3,CI2SAT
    2 FORMAT(2F10.1, 3E15.3)
      TEMPK = TEMPC + 273.16
      AK2 = EXP(-111.98 + 16.725*ALOG(TEMPK) + 6952.3/TEMPK)
      AK4 = 1.2E-11 + (3.6E-13)*(TEMPC - 25.)
      WRITE(51,4) TEMPC,PH,AK1,AK2,AK3,AK4,CI2SAT
    4 FORMAT(1H1 'RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULAT
     1IONS'/' TEMPERATURE = ',F5.1,' DEG C     PH = ' F3.1 /' K1 = ',1PE8
     2.2,' K2 = ', 1PE8.2, ' K3 = ', 1P E8.2, ' K4 = ',1PE8.2/' SOLUBILI
     3TY OF I2 IN WATER = ',1PE8.2, ' MOL/L' //54X'CONCENTRATIONS IN MOL
     4S/L' //
     5'  CONC I2 IN LIQ       CONC HIO        CONC H2OI+       CONC IODIDE
     6      CONC I3-   TOTAL I2 IN LIQ  LOG TOTAL I       PARTITION COEFF')
      CI2AQ = CI2SAT
      HIONC = EXP(-2.303*PH)
      DO 6  J = 1,40
      Y =  ((AK3*CI2AQ)/HIONC + AK4*CI2AQ)/(1. + AK2*CI2AQ)
      CIMIN = SQRT(Y)
      CI3 = AK2*CI2AQ*CIMIN
      CHIO = (AK3*CI2AQ)/(HIONC*CIMIN)
      CH2OI  = (AK4*CI2AQ)/CIMIN
      TOTCI2 = CI2AQ + 0.5*(CHIO + CH2OI + CIMIN + 3.*CI3)
      CI2G = CI2AQ/AK1
      P = TOTCI2/CI2G
      CLOG =ALOG(TOTCI2)/2.302585
      WRITE (51,5) CI2AQ,CHIO,CH2OI,CIMIN,CI3,TOTCI2,CLOG,P
    5 FORMAT (1P6E16.2,0PF16.3,1PE16.2)
      IF(TOTCI2.LT.1.E-9) GO TO 1
    6 CI2AQ = CI2AQ/2.
    1 CONTINUE
    3 STOP
      END
```

The second program deals with the case of iodate equilibrium. This involves including reaction 5 and Eq. (20) instead of Eq. (10). The key operation is solution of Eq. (22), a sixth power algebraic equation. For the 360 system, it turned out to be necessary to use Horner's method. This is a successive approximation procedure in which one starts with a fairly large interval containing a root, finds which half of the interval contains the root, and repeatedly halves the interval until the value of the root is known as closely as desired.

```
C CALCULATION OF PARTITION COEFFICIENT OF IODINE BETWEEN WATER AND AIR
      IMPLICIT REAL*8(A-H, O-Z  )
      DO 1 I = 1,100
      READ(50,2,END=3)TEMPC,PH,AK1,AK3,CI2SAT,AK5
    2 FORMAT (2F10.1,4E15.3)
      TEMPK = TEMPC + 273.16
      AK2 = EXP(-111.98 + 16.725*ALOG(TEMPK) + 6952.3/TEMPK)
      AK4 = 1.2E-11 + (3.6E-13)*(TEMPC - 25.)
      WRITE(51,4)TEMPC,PH,CI2SAT,AK1,AK2,AK3,AK4,AK5
    4 FORMAT(1H1,'CALCULATION OF PARTITION COEFFICIENT FOR IODINE BETWEE
     1N WATER AND AIR, ASSUMING EQUILIBRIUM IODATE FORMATION'//          '
     2 TEMPERATURE = ',F5.1,' DEG C              PH = ',F3.1,10X       'SATU
     3RATION CONC OF I2 IN LIQUID = ', 1PE10.3,' MOL/L' /                '
     4K1 = ',E10.2,'                  K2 = ',E10.2,'                  K3 = '
     5,E10.2/' K4 = ',E10.2,15X            'K5 = ',E10.2//54X'CONCENTRATIO
     6NS IN MOLS/L'//' CONC OF I2     CONC OF HIO    CONC OF H2OI+     CONC
     7 OF I-       CONC OF I3-     CONC OF IO3-    TOTAL I2 (AQ)  LOG C(I2)
     8  PART COEFF')
      N = 1
      X = 1.
      CI2AQ = CI2SAT
      HIONC = EXP(-2.303*PH)
      C4 = 5.*AK5/(HIONC**6)
   24 DO 6 J = 1,40
      C1 = 1. + AK2*CI2AQ
      C2 = AK3*CI2AQ/HIONC + AK4*CI2AQ
      C3 = C4*(CI2AQ**3)
      XLAST = 0.
   21 Y = (X + XLAST)/2.
      FOFX = C1*(X**6) - C2*(X**4) - C3
      IF(FOFX.LE.0.) GO TO 22
      FOFY = C1*(Y**6) - C2*(Y**4) - C3
      IF(FOFX.GT.0..AND.FOFY.LT.0..OR.FOFX.LT.0..AND.FOFY.GT.0.)GO TO 20
      IF(ABS((Y/X - 1.)).LT.1.E-5) GO TO 7
      X = Y
      IF (N.GT.99) GO TO 8
      N = N + 1
      GO TO 21
   20 IF(ABS((Y/X - 1.)).LT.1.E-5) GO TO 7
      XLAST = Y
      IF (N.GT.99) GO TO 8
      N = N + 1
      GO TO 21
    7 CIMIN = Y
      N = 1
      CI3 = AK2*CI2AQ*CIMIN
      CHIO = (AK3*CI2AQ)/(HIONC*CIMIN)
      CH2OI  = (AK4*CI2AQ)/CIMIN
      CIO3 = 0.2*(CIMIN + CI3 - CHIO - CH2OI)
      TOTCI2 = CI2AQ + 0.5*(CHIO + CH2OI + CIMIN + CIO3 + 3.*CI3)
      CI2G = CI2AQ/AK1
      P = TOTCI2/CI2G
      CLOG =ALOG(TOTCI2)/2.302585
      WRITE(51,11) CI2AQ,CHIO,CH2OI,CIMIN,CI3,CIO3,TOTCI2,CLOG,P
   11 FORMAT(1PE10.3, 6E15.3, 0PF13.3, 1PE15.3)
      IF(TOTCI2.LT.1.E-9) GO TO 1
    6 CI2AQ = CI2AQ/2.
   22 X = 2.*X
      IF(X.GT.40.) GO TO 23
      GO TO 24
   23 CI2AQ = CI2AQ/2.
      GO TO 24
    8 WRITE(51,9)
    9 FORMAT(//' THERE WERE MORE THAN 99 ITERATIONS IN THE SOLUTION FOR
     1X ')
      GO TO 1
    3 STOP
      END
```

The third variation incorporates the volatile HIO case. This involves including Eq. (9) in the computation and replacing Eq. (10) by Eq. (24). The values of K_9 and the gas-to-liquid volume ratio are incorporated in the input. As in the first case, the algebra is straightforward.

```
C CALCULATION OF PARTITION COEFFICIENT OF IODINE BETWEEN WATER AND AIR
      DO 1 I = 1,100
      READ(50,2,END=3) TEMPC,PH,AK1,AK3,CI2SAT,AK5,VGVL
    2 FORMAT(2F10.1,5E10.3)
      TEMPK = TEMPC + 273.16
      AK2 = EXP(-111.98 + 16.725*ALOG(TEMPK) + 6952.3/TEMPK)
      AK4 = 1.2E-11 + (3.6E-13)*(TEMPC - 25.)
      WRITE(51,4) TEMPC,PH,AK1,AK2,AK3,AK4,AK5,VGVL
    4 FORMAT(1H1 'RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULAT
     1IONS, INCLUDING EFFECT OF HCI VOLATILITY'//' TEMPERATURE =',F5.1,'
     2 DEG C      PH =',F3.1/' K1 =',1PE8.2,'      K2 =', E8.2,'      K3 ='
     3,E8.2/' K4 =',E8.2, '      K5 =',E8.2/' RATIO OF GAS VOLUME TO LIQU
     4ID VOLUME =',E8.2//54X'CONCENTRATIONS IN MOLS/L'//                '
     5 CONC OF I2  CONC OF I2  CONC HIO    CONC OF      CONC OF I-  CONC
     6OF      CONC OF HIO TOTAL I IN  TOTAL I IN LOG TOTAL   PARTITION'/'
     7  IN GAS      IN LIQUID   IN LIQUID   H2/I+ (AQ)                 I3
     8-       IN GAS      LIQUID        GAS       I (AQ)     COEFFICIENT')
      CI2AQ = CI2SAT
      HIONC = EXP(-2.303*PH)
      A = 1. + VGVL/AK5
      DO 6  J = 1,40
      Y = (A*AK3*CI2AQ/HIONC + AK4*CI2AQ)/(1. + AK2*CI2AQ)
      CIMIN = SQRT(Y)
      CI3 = AK2*CI2AQ*CIMIN
      CHIO = (AK3*CI2AQ)/(HIONC*CIMIN)
      CH2OI  = (AK4*CI2AQ)/CIMIN
      TOTCI2 = CI2AQ + 0.5*(CHIO + CH2OI + CIMIN + 3.*CI3)
      CI2G = CI2AQ/AK1
      CHIOG = CHIO/AK5
      CG = CI2G + 0.5*CHIOG
      P = TOTCI2/CG
      CLOG =ALOG(TOTCI2)/2.302585
      WRITE(51,5)CI2G,CI2AQ,CHIO,CH2OI,CIMIN,CI3,CHIOG,TOTCI2,CG,CLOG,P
    5 FORMAT(1P9E12.2,0PF9.3,1PE12.2)
      IF(TOTCI2.LT.1.E-9) GO TO 1
    6 CI2AQ = CI2AQ/2.
    1 CONTINUE
    3 STOP
      END
```

Table 1. Solubility and Vapor Pressure Data and Calculation of K_1

t, Temperature (°C)	Solubility (g/liter)	C_l, Solubility (moles/liter)	P, Vapor Pressure (mm Hg)	C_g, Vapor Concentration (moles/liter)	$K_1 = C_l/C_g$
0	0.14	5.51×10^{-4}	2.99×10^{-2}	1.75×10^{-6}	315
10	0.20	7.87×10^{-4}	8.08×10^{-2}	4.56×10^{-6}	173
20	0.285	1.12×10^{-3}	2.02×10^{-1}	1.10×10^{-5}	102
25	0.336	1.32×10^{-3}	3.3×10^{-1}	1.77×10^{-5}	74.6
30	0.385	1.52×10^{-3}	4.71×10^{-1}	2.49×10^{-5}	61.0
40	0.52	2.05×10^{-3}	1.03	5.26×10^{-5}	39.0
50	0.71	2.80×10^{-3}	2.16	1.07×10^{-4}	26.2
60	1.00	3.94×10^{-3}	4.31	2.07×10^{-4}	19.0
70	1.50	5.90×10^{-3}	8.22	3.83×10^{-4}	15.4
80	2.25	8.86×10^{-3}	15.1	6.84×10^{-4}	13.0
90	3.15	1.24×10^{-2}	26.8	1.18×10^{-3}	10.5
100	4.45	1.75×10^{-2}	45.5	1.95×10^{-3}	9.0
106	5.60	2.20×10^{-2}	62	2.62×10^{-3}	8.40
110	6.6	2.60×10^{-2}	74.5	3.11×10^{-3}	8.36
112.3	7.20	2.83×10^{-2}	82	3.40×10^{-3}	8.32
120		3.25×10^{-2}	112	4.55×10^{-3}	7.14
130		3.98×10^{-2}	157	6.25×10^{-3}	6.37
140		4.98×10^{-2}	216	8.37×10^{-3}	5.95
150		6.22×10^{-2}	297	1.13×10^{-2}	5.52

Table 2. K_3 vs Temperature

Temperature (°C)	K_3
0	4.1×10^{-14}
10	1.2×10^{-13}
20	3.4×10^{-13}
25	5.4×10^{-13}
30	8.4×10^{-13}
40	2.1×10^{-12}
50	4.8×10^{-12}
60	1.0×10^{-11}
70	2.2×10^{-11}
80	4.3×10^{-11}
90	8.4×10^{-11}
100	1.5×10^{-10}
105	2.1×10^{-10}
110	2.7×10^{-10}
120	4.8×10^{-10}
130	7.8×10^{-10}
140	1.2×10^{-9}
150	2.0×10^{-9}

Table 3. Results of Calculations, t = 25°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 5.0
K1 = 7.46E 01 K2 = 7.58E 02 K3 = 5.40E-13 K4 = 1.20E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	1.20E-05	2.65E-09	5.98E-06	5.98E-06	1.34E-03	-2.874	7.56E 01
6.60E-04	7.32E-06	1.62E-09	4.88E-06	2.44E-06	6.70E-04	-3.174	7.57E 01
3.30E-04	4.72E-06	1.05E-09	3.78E-06	9.45E-07	3.36E-04	-3.474	7.59E 01
1.65E-04	3.17E-06	7.03E-10	2.82E-06	3.52E-07	1.69E-04	-3.773	7.62E 01
8.25E-05	2.18E-06	4.83E-10	2.05E-06	1.28E-07	8.48E-05	-4.072	7.67E 01
4.12E-05	1.52E-06	3.36E-10	1.47E-06	4.60E-08	4.28E-05	-4.368	7.74E 01
2.06E-05	1.06E-06	2.36E-10	1.05E-06	1.64E-08	2.17E-05	-4.663	7.85E 01
1.03E-05	7.50E-07	1.66E-10	7.44E-07	5.81E-09	1.11E-05	-4.956	8.01E 01
5.16E-06	5.29E-07	1.17E-10	5.27E-07	2.06E-09	5.69E-06	-5.245	8.23E 01
2.58E-06	3.74E-07	8.29E-11	3.73E-07	7.29E-10	2.95E-06	-5.530	8.54E 01
1.29E-06	2.64E-07	5.86E-11	2.64E-07	2.58E-10	1.55E-06	-5.809	8.99E 01
6.45E-07	1.87E-07	4.14E-11	1.87E-07	9.12E-11	8.31E-07	-6.080	9.62E 01
3.22E-07	1.32E-07	2.93E-11	1.32E-07	3.22E-11	4.54E-07	-6.343	1.05E 02
1.61E-07	9.34E-08	2.07E-11	9.34E-08	1.14E-11	2.55E-07	-6.594	1.18E 02
8.06E-08	6.60E-08	1.46E-11	6.60E-08	4.03E-12	1.47E-07	-6.834	1.36E 02
4.03E-08	4.67E-08	1.04E-11	4.67E-08	1.42E-12	8.70E-08	-7.061	1.61E 02
2.01E-08	3.30E-08	7.32E-12	3.30E-08	5.04E-13	5.32E-08	-7.274	1.97E 02
1.01E-08	2.33E-08	5.18E-12	2.33E-08	1.78E-13	3.34E-08	-7.476	2.48E 02
5.04E-09	1.65E-08	3.66E-12	1.65E-08	6.30E-14	2.15E-08	-7.667	3.19E 02
2.52E-09	1.17E-08	2.59E-12	1.17E-08	2.23E-14	1.42E-08	-7.848	4.20E 02
1.26E-09	8.25E-09	1.83E-12	8.25E-09	7.87E-15	9.51E-09	-8.022	5.64E 02
6.29E-10	5.84E-09	1.29E-12	5.84E-09	2.78E-15	6.47E-09	-8.189	7.66E 02
3.15E-10	4.13E-09	9.15E-13	4.13E-09	9.84E-16	4.44E-09	-8.352	1.05E 03
1.57E-10	2.92E-09	6.47E-13	2.92E-09	3.48E-16	3.08E-09	-8.512	1.46E 03
7.87E-11	2.06E-09	4.58E-13	2.06E-09	1.23E-16	2.14E-09	-8.669	2.03E 03
3.93E-11	1.46E-09	3.24E-13	1.46E-09	4.35E-17	1.50E-09	-8.824	2.84E 03
1.97E-11	1.03E-09	2.29E-13	1.03E-09	1.54E-17	1.05E-09	-8.978	3.99E 03
9.83E-12	7.29E-10	1.62E-13	7.30E-10	5.44E-18	7.39E-10	-9.131	5.61E 03

Table 4. Results of Calculations, t = 25°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 7.0
K1 = 7.46E 01 K2 = 7.58E 02 K3 = 5.40E-13 K4 = 1.20E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	1.20E-04	2.65E-10	5.98E-05	5.98E-05	1.50E-03	-2.824	8.47E 01
6.60E-04	7.32E-05	1.62E-10	4.88E-05	2.44E-05	7.58E-04	-3.121	8.56E 01
3.30E-04	4.73E-05	1.05E-10	3.78E-05	9.45E-06	3.87E-04	-3.413	8.74E 01
1.65E-04	3.17E-05	7.03E-11	2.82E-05	3.52E-06	2.00E-04	-3.698	9.05E 01
8.25E-05	2.18E-05	4.83E-11	2.05E-05	1.28E-06	1.06E-04	-3.976	9.55E 01
4.12E-05	1.52E-05	3.36E-11	1.47E-05	4.60E-07	5.69E-05	-4.245	1.03E 02
2.06E-05	1.07E-05	2.36E-11	1.05E-05	1.64E-07	3.14E-05	-4.503	1.14E 02
1.03E-05	7.50E-06	1.66E-11	7.44E-06	5.82E-08	1.79E-05	-4.748	1.29E 02
5.16E-06	5.29E-06	1.17E-11	5.27E-06	2.06E-08	1.05E-05	-4.980	1.52E 02
2.58E-06	3.74E-06	8.29E-12	3.73E-06	7.29E-09	6.33E-06	-5.199	1.83E 02
1.29E-06	2.64E-06	5.86E-12	2.64E-06	2.58E-09	3.94E-06	-5.405	2.28E 02
6.45E-07	1.87E-06	4.14E-12	1.87E-06	9.12E-10	2.51E-06	-5.600	2.91E 02
3.22E-07	1.32E-06	2.93E-12	1.32E-06	3.22E-10	1.64E-06	-5.784	3.81E 02
1.61E-07	9.34E-07	2.07E-12	9.34E-07	1.14E-10	1.10E-06	-5.960	5.07E 02
8.06E-08	6.61E-07	1.46E-12	6.61E-07	4.03E-11	7.41E-07	-6.130	6.86E 02
4.03E-08	4.67E-07	1.03E-12	4.67E-07	1.43E-11	5.07E-07	-6.295	9.40E 02
2.01E-08	3.30E-07	7.32E-13	3.30E-07	5.04E-12	3.50E-07	-6.455	1.30E 03
1.01E-08	2.34E-07	5.17E-13	2.34E-07	1.78E-12	2.44E-07	-6.613	1.80E 03
5.04E-09	1.65E-07	3.66E-13	1.65E-07	6.30E-13	1.70E-07	-6.769	2.52E 03
2.52E-09	1.17E-07	2.59E-13	1.17E-07	2.23E-13	1.19E-07	-6.923	3.53E 03
1.26E-09	8.26E-08	1.83E-13	8.26E-08	7.87E-14	8.38E-08	-7.077	4.97E 03
6.29E-10	5.84E-08	1.29E-13	5.84E-08	2.78E-14	5.90E-08	-7.229	6.99E 03
3.15E-10	4.13E-08	9.15E-14	4.13E-08	9.84E-15	4.16E-08	-7.381	9.86E 03
1.57E-10	2.92E-08	6.47E-14	2.92E-08	3.48E-15	2.93E-08	-7.532	1.39E 04
7.87E-11	2.06E-08	4.57E-14	2.06E-08	1.23E-15	2.07E-08	-7.684	1.96E 04
3.93E-11	1.46E-08	3.23E-14	1.46E-08	4.35E-16	1.46E-08	-7.835	2.78E 04
1.97E-11	1.03E-08	2.29E-14	1.03E-08	1.54E-16	1.03E-08	-7.985	3.92E 04
9.83E-12	7.30E-09	1.62E-14	7.30E-09	5.44E-17	7.31E-09	-8.136	5.54E 04
4.92E-12	5.16E-09	1.14E-14	5.16E-09	1.92E-17	5.17E-09	-8.287	7.84E 04
2.46E-12	3.65E-09	8.09E-15	3.65E-09	6.80E-18	3.65E-09	-8.438	1.11E 05
1.23E-12	2.58E-09	5.72E-15	2.58E-09	2.40E-18	2.58E-09	-8.588	1.57E 05
6.15E-13	1.82E-09	4.04E-15	1.82E-09	8.50E-19	1.83E-09	-8.739	2.22E 05
3.07E-13	1.29E-09	2.86E-15	1.29E-09	3.00E-19	1.29E-09	-8.889	3.13E 05
1.54E-13	9.12E-10	2.02E-15	9.12E-10	1.06E-19	9.12E-10	-9.040	4.43E 05

Table 5. Results of Calculations, t = 25°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 8.0
K1 = 7.46E-01 K2 = 7.58E-02 K3 = 5.4[illegible]E-13 K+ = 1.2[illegible]E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	3.78E-04	5.38E-11	1.89E-04	1.89E-04	1.89E-03	-2.724	1.07E 02
5.67E-04	2.32E-04	5.13E-11	1.94E-04	7.72E-05	9.69E-04	-3.014	1.10E 02
3.37E-04	1.49E-04	5.31E-11	1.20E-04	2.99E-05	5.09E-04	-3.293	1.15E 02
1.65E-04	1.[illegible]E-04	2.22E-11	5.91E-05	1.11E-05	2.76E-04	-3.558	1.25E 02
8.25E-05	5.89E-05	1.53E-11	5.49E-05	4.05E-06	1.55E-04	-3.808	1.41E 02
4.12E-05	4.8[illegible]E-05	1.0[illegible]E-11	4.90E-05	1.45E-06	9.07E-05	-4.042	1.64E 02
2.[illegible]6E-05	3.37E-05	7.46E-12	3.92E-05	5.18E-07	5.48E-05	-4.261	1.98E 02
1.[illegible]3E-05	2.37E-05	5.20E-12	2.35E-05	1.84E-07	3.42E-05	-4.466	2.48E 02
5.16E-06	1.67E-05	3.71E-12	1.67E-05	6.52E-08	2.20E-05	-4.658	3.18E 02
2.58E-06	1.18E-05	2.62E-12	1.18E-05	2.31E-08	1.44E-05	-4.841	4.18E 02
1.29E-06	8.30E-06	1.85E-12	8.35E-06	8.16E-09	9.66E-06	-5.015	5.59E 02
6.45E-07	5.91E-06	1.31E-12	5.91E-06	2.88E-09	6.56E-06	-5.183	7.59E 02
3.22E-07	4.18E-06	9.25E-13	4.18E-06	1.02E-09	4.50E-06	-5.347	1.04E 03
1.61E-07	2.95E-06	6.54E-13	2.95E-06	3.61E-10	3.12E-06	-5.506	1.44E 03
8.06E-08	2.[illegible]9E-06	4.63E-13	2.09E-06	1.28E-10	2.17E-06	-5.664	2.01E 03
4.03E-08	1.48E-06	3.27E-13	1.48E-06	4.51E-11	1.52E-06	-5.819	2.81E 03
2.01E-08	1.04E-06	2.31E-13	1.04E-06	1.59E-11	1.06E-06	-5.973	3.94E 03
1.01E-08	7.39E-07	1.64E-13	7.39E-07	5.64E-12	7.49E-07	-6.126	5.55E 03
5.04E-09	5.22E-07	1.16E-13	5.22E-07	1.99E-12	5.27E-07	-6.278	7.81E 03
2.52E-09	3.69E-07	8.18E-14	3.69E-07	7.04E-13	3.72E-07	-6.430	1.10E 04
1.26E-09	2.61E-07	5.78E-14	2.61E-07	2.49E-13	2.62E-07	-6.581	1.56E 04
6.29E-10	1.85E-07	4.09E-14	1.85E-07	8.81E-14	1.85E-07	-6.732	2.20E 04
3.15E-10	1.31E-07	2.89E-14	1.31E-07	3.11E-14	1.31E-07	-6.883	3.10E 04
1.57E-10	9.23E-08	2.05E-14	9.23E-08	1.10E-14	9.25E-08	-7.034	4.38E 04
7.87E-11	6.53E-08	1.45E-14	6.53E-08	3.89E-15	6.54E-08	-7.185	6.20E 04
3.93E-11	4.62E-08	1.02E-14	4.62E-08	1.38E-15	4.62E-08	-7.335	8.76E 04
1.97E-11	3.26E-08	7.23E-15	3.26E-08	4.86E-16	3.27E-08	-7.486	1.24E 05
9.83E-12	2.31E-08	5.11E-15	2.31E-08	1.72E-16	2.31E-08	-7.637	1.75E 05
4.92E-12	1.63E-08	3.62E-15	1.63E-08	6.08E-17	1.63E-08	-7.787	2.48E 05
2.46E-12	1.15E-08	2.55E-15	1.15E-08	2.15E-17	1.15E-08	-7.938	3.50E 05
1.23E-12	8.16E-09	1.81E-15	8.16E-09	7.60E-18	8.16E-09	-8.088	4.95E 05
6.15E-13	5.77E-09	1.28E-15	5.77E-09	2.69E-18	5.77E-09	-8.239	7.00E 05
3.07E-13	4.08E-09	9.04E-16	4.08E-09	9.50E-19	4.08E-09	-8.389	9.91E 05
1.54E-13	2.89E-09	6.39E-16	2.89E-09	3.36E-19	2.89E-09	-8.540	1.40E 06
7.68E-14	2.04E-09	4.52E-16	2.04E-09	1.19E-19	2.04E-09	-8.690	1.98E 06
3.84E-14	1.44E-09	3.20E-16	1.44E-09	4.20E-20	1.44E-09	-8.841	2.80E 06
1.92E-14	1.02E-09	2.26E-16	1.02E-09	1.48E-20	1.02E-09	-8.991	3.96E 06
9.6[illegible]E-15	7.21E-1[illegible]	1.59E-16	7.21E-10	5.25E-21	7.21E-10	-9.142	5.60E 06

Table 6. Results of Calculations, t = 25°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 9.0
K1 = 7.46E-01 K2 = 7.58E-02 K3 = 5.40E-13 K4 = 1.20E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	1.20E-03	2.65E-11	5.98E-04	5.98E-04	3.11E-03	-2.507	1.76E 02
6.60E-04	7.33E-04	1.62E-11	4.88E-04	2.44E-04	1.64E-03	-2.786	1.85E 02
3.30E-04	4.73E-04	1.05E-11	3.78E-04	9.46E-05	8.97E-04	-3.047	2.03E 02
1.65E-04	3.17E-04	7.02E-12	2.82E-04	3.52E-05	5.17E-04	-3.286	2.34E 02
8.25E-05	2.18E-04	4.83E-12	2.05E-04	1.28E-05	3.13E-04	-3.504	2.83E 02
4.12E-05	1.52E-04	3.36E-12	1.47E-04	4.60E-06	1.98E-04	-3.704	3.58E 02
2.06E-05	1.07E-04	2.36E-12	1.05E-04	1.64E-06	1.29E-04	-3.890	4.66E 02
1.03E-05	7.51E-05	1.66E-12	7.45E-05	5.82E-07	8.59E-05	-4.066	6.22E 02
5.16E-06	5.30E-05	1.17E-12	5.28E-05	2.06E-07	5.83E-05	-4.234	8.44E 02
2.58E-06	3.74E-05	8.28E-13	3.73E-05	7.29E-08	4.01E-05	-4.397	1.16E 03
1.29E-06	2.64E-05	5.85E-13	2.64E-05	2.58E-08	2.78E-05	-4.557	1.61E 03
6.45E-07	1.87E-05	4.14E-13	1.87E-05	9.12E-09	1.93E-05	-4.713	2.24E 03
3.22E-07	1.32E-05	2.93E-13	1.32E-05	3.23E-09	1.35E-05	-4.868	3.14E 03
1.61E-07	9.35E-06	2.07E-13	9.34E-06	1.14E-09	9.51E-06	-5.022	4.40E 03
8.06E-08	6.61E-06	1.46E-13	6.61E-06	4.03E-10	6.69E-06	-5.175	6.19E 03
4.03E-08	4.67E-06	1.03E-13	4.67E-06	1.43E-10	4.71E-06	-5.327	8.73E 03
2.01E-08	3.30E-06	7.32E-14	3.30E-06	5.04E-11	3.32E-06	-5.478	1.23E 04
1.01E-08	2.34E-06	5.17E-14	2.34E-06	1.78E-11	2.35E-06	-5.630	1.74E 04
5.04E-09	1.65E-06	3.66E-14	1.65E-06	6.30E-12	1.66E-06	-5.781	2.45E 04
2.52E-09	1.17E-06	2.59E-14	1.17E-06	2.23E-12	1.17E-06	-5.932	3.47E 04
1.26E-09	8.26E-07	1.83E-14	8.26E-07	7.88E-13	8.27E-07	-6.082	4.90E 04
6.29E-10	5.84E-07	1.29E-14	5.84E-07	2.79E-13	5.85E-07	-6.233	6.93E 04
3.15E-10	4.13E-07	9.14E-15	4.13E-07	9.85E-14	4.13E-07	-6.384	9.80E 04
1.57E-10	2.92E-07	6.47E-15	2.92E-07	3.48E-14	2.92E-07	-6.534	1.39E 05
7.87E-11	2.07E-07	4.57E-15	2.07E-07	1.23E-14	2.07E-07	-6.685	1.96E 05
3.93E-11	1.46E-07	3.23E-15	1.46E-07	4.35E-15	1.46E-07	-6.835	2.77E 05
1.97E-11	1.03E-07	2.29E-15	1.03E-07	1.54E-15	1.03E-07	-6.986	3.92E 05
9.83E-12	7.30E-08	1.62E-15	7.30E-08	5.44E-16	7.30E-08	-7.137	5.54E 05
4.92E-12	5.16E-08	1.14E-15	5.16E-08	1.92E-16	5.16E-08	-7.287	7.83E 05
2.46E-12	3.65E-08	8.08E-16	3.65E-08	6.80E-17	3.65E-08	-7.438	1.11E 06
1.23E-12	2.58E-08	5.71E-16	2.58E-08	2.40E-17	2.58E-08	-7.588	1.57E 06
6.15E-13	1.83E-08	4.04E-16	1.83E-08	8.50E-18	1.83E-08	-7.739	2.22E 06
3.07E-13	1.29E-08	2.86E-16	1.29E-08	3.01E-18	1.29E-08	-7.889	3.13E 06
1.54E-13	9.13E-09	2.02E-16	9.13E-09	1.06E-18	9.13E-09	-8.040	4.43E 06
7.68E-14	6.45E-09	1.43E-16	6.45E-09	3.76E-19	6.45E-09	-8.190	6.27E 06
3.84E-14	4.56E-09	1.01E-16	4.56E-09	1.33E-19	4.56E-09	-8.341	8.86E 06
1.92E-14	3.23E-09	7.14E-17	3.23E-09	4.70E-20	3.23E-09	-8.491	1.25E 07
9.60E-15	2.28E-09	5.05E-17	2.28E-09	1.66E-20	2.28E-09	-8.642	1.77E 07
4.80E-15	1.61E-09	3.57E-17	1.61E-09	5.87E-21	1.61E-09	-8.792	2.51E 07
2.40E-15	1.14E-09	2.53E-17	1.14E-09	2.08E-21	1.14E-09	-8.943	3.54E 07

Table 7. Results of Calculations, t = 25°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 9.2
K1 = 7.46E 01 K2 = 7.58E 02 K3 = 5.40E-13 K4 = 1.20E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	1.51E-03	2.10E-11	7.53E-04	7.53E-04	3.58E-03	-2.446	2.02E 02
6.60E-04	9.22E-04	1.29E-11	6.15E-04	3.07E-04	1.89E-03	-2.724	2.14E 02
3.30E-04	5.95E-04	8.32E-12	4.76E-04	1.19E-04	1.04E-03	-2.981	2.36E 02
1.65E-04	3.99E-04	5.58E-12	3.55E-04	4.44E-05	6.09E-04	-3.216	2.75E 02
8.25E-05	2.74E-04	3.83E-12	2.58E-04	1.61E-05	3.73E-04	-3.428	3.37E 02
4.12E-05	1.91E-04	2.67E-12	1.85E-04	5.79E-06	2.38E-04	-3.623	4.31E 02
2.06E-05	1.34E-04	1.87E-12	1.32E-04	2.06E-06	1.57E-04	-3.805	5.67E 02
1.03E-05	9.45E-05	1.32E-12	9.38E-05	7.33E-07	1.06E-04	-3.977	7.63E 02
5.16E-06	6.67E-05	9.31E-13	6.64E-05	2.59E-07	7.21E-05	-4.142	1.04E 03
2.58E-06	4.71E-05	6.58E-13	4.70E-05	9.18E-08	4.98E-05	-4.303	1.44E 03
1.29E-06	3.33E-05	4.65E-13	3.33E-05	3.25E-08	3.46E-05	-4.461	2.00E 03
6.45E-07	2.35E-05	3.29E-13	2.35E-05	1.15E-08	2.42E-05	-4.616	2.80E 03
3.22E-07	1.66E-05	2.32E-13	1.66E-05	4.06E-09	1.70E-05	-4.770	3.93E 03
1.61E-07	1.18E-05	1.64E-13	1.18E-05	1.44E-09	1.19E-05	-4.923	5.52E 03
8.06E-08	8.32E-06	1.16E-13	8.32E-06	5.08E-10	8.40E-06	-5.076	7.78E 03
4.03E-08	5.88E-06	8.22E-14	5.88E-06	1.80E-10	5.92E-06	-5.227	1.10E 04
2.01E-08	4.16E-06	5.81E-14	4.16E-06	6.35E-11	4.18E-06	-5.379	1.55E 04
1.01E-08	2.94E-06	4.11E-14	2.94E-06	2.24E-11	2.95E-06	-5.530	2.19E 04
5.04E-09	2.08E-06	2.91E-14	2.08E-06	7.93E-12	2.08E-06	-5.681	3.09E 04
2.52E-09	1.47E-06	2.05E-14	1.47E-06	2.81E-12	1.47E-06	-5.832	4.37E 04
1.26E-09	1.04E-06	1.45E-14	1.04E-06	9.92E-13	1.04E-06	-5.982	6.17E 04
6.29E-10	7.35E-07	1.03E-14	7.35E-07	3.51E-13	7.36E-07	-6.133	8.72E 04
3.15E-10	5.20E-07	7.26E-15	5.20E-07	1.24E-13	5.20E-07	-6.284	1.23E 05
1.57E-10	3.68E-07	5.14E-15	3.68E-07	4.38E-14	3.68E-07	-6.434	1.74E 05
7.87E-11	2.60E-07	3.63E-15	2.60E-07	1.55E-14	2.60E-07	-6.585	2.47E 05
3.93E-11	1.84E-07	2.57E-15	1.84E-07	5.48E-15	1.84E-07	-6.735	3.49E 05
1.97E-11	1.30E-07	1.82E-15	1.30E-07	1.94E-15	1.30E-07	-6.886	4.93E 05
9.83E-12	9.19E-08	1.28E-15	9.19E-08	6.85E-16	9.19E-08	-7.037	6.97E 05
4.92E-12	6.50E-08	9.08E-16	6.50E-08	2.42E-16	6.50E-08	-7.187	9.86E 05
2.46E-12	4.60E-08	6.42E-16	4.60E-08	8.56E-17	4.60E-08	-7.338	1.39E 06
1.23E-12	3.25E-08	4.54E-16	3.25E-08	3.03E-17	3.25E-08	-7.488	1.97E 06
6.15E-13	2.30E-08	3.21E-16	2.30E-08	1.07E-17	2.30E-08	-7.639	2.79E 06
3.07E-13	1.62E-08	2.27E-16	1.62E-08	3.78E-18	1.62E-08	-7.789	3.94E 06
1.54E-13	1.15E-08	1.60E-16	1.15E-08	1.34E-18	1.15E-08	-7.940	5.58E 06
7.68E-14	8.12E-09	1.13E-16	8.12E-09	4.73E-19	8.12E-09	-8.090	7.89E 06
3.84E-14	5.74E-09	8.02E-17	5.74E-09	1.67E-19	5.74E-09	-8.241	1.12E 07
1.92E-14	4.06E-09	5.67E-17	4.06E-09	5.91E-20	4.06E-09	-8.391	1.58E 07
9.60E-15	2.87E-09	4.01E-17	2.87E-09	2.09E-20	2.87E-09	-8.542	2.23E 07
4.80E-15	2.03E-09	2.84E-17	2.03E-09	7.39E-21	2.03E-09	-8.692	3.16E 07
2.40E-15	1.44E-09	2.01E-17	1.44E-09	2.61E-21	1.44E-09	-8.843	4.46E 07

Table 8. Results of Calculations, t = 25°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 25.0 DEG C PH = 9.5
K1 = 7.46E-01 K2 = 7.68E-02 K3 = 5.42E-13 K4 = 1.20E-11
SOLUBILITY OF I2 IN WATER = 1.32E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.32E-03	2.13E-03	1.49E-11	1.06E-03	1.06E-03	4.51E-03	-2.346	2.55E 02
6.60E-04	1.30E-03	9.12E-12	8.69E-04	4.34E-04	2.40E-03	-2.620	2.71E 02
3.30E-04	8.41E-04	5.89E-12	6.73E-04	1.68E-04	1.34E-03	-2.873	3.03E 02
1.65E-04	5.64E-04	3.95E-12	5.01E-04	6.27E-05	7.92E-04	-3.101	3.58E 02
8.25E-05	3.88E-04	2.71E-12	3.65E-04	2.28E-05	4.93E-04	-3.307	4.46E 02
4.12E-05	2.70E-04	1.89E-12	2.62E-04	8.18E-06	3.19E-04	-3.496	5.78E 02
2.06E-05	1.93E-04	1.33E-12	1.87E-04	2.92E-06	2.13E-04	-3.672	7.71E 02
1.03E-05	1.33E-04	9.34E-13	1.32E-04	1.03E-06	1.45E-04	-3.839	1.05E 03
5.16E-06	9.42E-05	6.59E-13	9.38E-05	3.67E-07	9.97E-05	-4.001	1.44E 03
2.58E-06	6.65E-05	4.66E-13	6.64E-05	1.30E-07	6.93E-05	-4.160	2.00E 03
1.29E-06	4.70E-05	3.29E-13	4.70E-05	4.59E-08	4.84E-05	-4.315	2.80E 03
6.45E-07	3.32E-05	2.33E-13	3.32E-05	1.62E-08	3.39E-05	-4.470	3.92E 03
3.22E-07	2.35E-05	1.65E-13	2.35E-05	5.74E-09	2.38E-05	-4.623	5.52E 03
1.61E-07	1.66E-05	1.16E-13	1.66E-05	2.03E-09	1.68E-05	-4.775	7.77E 03
8.06E-08	1.18E-05	8.23E-14	1.18E-05	7.17E-10	1.18E-05	-4.927	1.10E 04
4.03E-08	8.31E-06	5.82E-14	8.31E-06	2.54E-10	8.35E-06	-5.078	1.55E 04
2.01E-08	5.88E-06	4.11E-14	5.88E-06	8.97E-11	5.90E-06	-5.229	2.18E 04
1.01E-08	4.16E-06	2.91E-14	4.16E-06	3.17E-11	4.17E-06	-5.380	3.09E 04
5.04E-09	2.94E-06	2.06E-14	2.94E-06	1.12E-11	2.94E-06	-5.531	4.36E 04
2.52E-09	2.08E-06	1.45E-14	2.08E-06	3.96E-12	2.08E-06	-5.682	6.16E 04
1.26E-09	1.47E-06	1.03E-14	1.47E-06	1.40E-12	1.47E-06	-5.833	8.71E 04
6.29E-10	1.04E-06	7.27E-15	1.04E-06	4.95E-13	1.04E-06	-5.983	1.23E 05
3.15E-10	7.35E-07	5.14E-15	7.35E-07	1.75E-13	7.35E-07	-6.134	1.74E 05
1.57E-10	5.19E-07	3.64E-15	5.19E-07	6.19E-14	5.20E-07	-6.284	2.46E 05
7.87E-11	3.67E-07	2.57E-15	3.67E-07	2.19E-14	3.67E-07	-6.435	3.48E 05
3.93E-11	2.60E-07	1.82E-15	2.60E-07	7.74E-15	2.60E-07	-6.585	4.93E 05
1.97E-11	1.84E-07	1.29E-15	1.84E-07	2.74E-15	1.84E-07	-6.736	6.97E 05
9.83E-12	1.30E-07	9.09E-16	1.30E-07	9.67E-16	1.30E-07	-6.887	9.85E 05
4.92E-12	9.18E-08	6.43E-16	9.18E-08	3.42E-16	9.18E-08	-7.037	1.39E 06
2.46E-12	6.49E-08	4.54E-16	6.49E-08	1.21E-16	6.49E-08	-7.188	1.97E 06
1.23E-12	4.59E-08	3.21E-16	4.59E-08	4.28E-17	4.59E-08	-7.338	2.79E 06
6.15E-13	3.25E-08	2.27E-16	3.25E-08	1.51E-17	3.25E-08	-7.489	3.94E 06
3.07E-13	2.30E-08	1.61E-16	2.30E-08	5.34E-18	2.30E-08	-7.639	5.57E 06
1.54E-13	1.62E-08	1.14E-16	1.62E-08	1.89E-18	1.62E-08	-7.790	7.88E 06
7.68E-14	1.15E-08	8.03E-17	1.15E-08	6.68E-19	1.15E-08	-7.940	1.11E 07
3.84E-14	8.12E-09	5.68E-17	8.12E-09	2.36E-19	8.12E-09	-8.091	1.58E 07
1.92E-14	5.74E-09	4.02E-17	5.74E-09	8.35E-20	5.74E-09	-8.241	2.23E 07
9.60E-15	4.06E-09	2.84E-17	4.06E-09	2.95E-20	4.06E-09	-8.392	3.15E 07
4.80E-15	2.87E-09	2.01E-17	2.87E-09	1.04E-20	2.87E-09	-8.542	4.46E 07
2.40E-15	2.03E-09	1.42E-17	2.03E-09	3.69E-21	2.03E-09	-8.693	6.30E 07

Table 9. Results of Calculations, t = 50°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 5.0
K1 = 2.62E-01 K2 = 4.80E-02 K3 = 4.80E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	5.62E-05	2.45E-09	2.40E-05	3.22E-05	2.89E-03	-2.539	2.70E 01
1.40E-03	3.35E-05	1.46E-09	2.01E-05	1.35E-05	1.45E-03	-2.840	2.71E 01
7.00E-04	2.12E-05	9.26E-10	1.59E-05	5.33E-06	7.27E-04	-3.139	2.72E 01
3.50E-04	1.40E-05	6.12E-10	1.20E-05	2.02E-06	3.66E-04	-3.436	2.74E 01
1.75E-04	9.55E-06	4.17E-10	8.81E-06	7.40E-07	1.85E-04	-3.732	2.77E 01
8.75E-05	6.62E-06	2.89E-10	6.36E-06	2.67E-07	9.44E-05	-4.025	2.83E 01
4.37E-05	4.64E-06	2.02E-10	4.54E-06	9.53E-08	4.85E-05	-4.314	2.90E 01
2.19E-05	3.26E-06	1.42E-10	3.23E-06	3.39E-08	2.52E-05	-4.599	3.01E 01
1.09E-05	2.30E-06	1.00E-10	2.29E-06	1.20E-08	1.32E-05	-4.878	3.17E 01
5.47E-06	1.62E-06	7.09E-11	1.62E-06	4.25E-09	7.10E-06	-5.149	3.40E 01
2.73E-06	1.15E-06	5.01E-11	1.15E-06	1.50E-09	3.88E-06	-5.411	3.72E 01
1.37E-06	8.11E-07	3.54E-11	8.11E-07	5.32E-10	2.18E-06	-5.662	4.18E 01
6.84E-07	5.73E-07	2.50E-11	5.73E-07	1.88E-10	1.26E-06	-5.901	4.82E 01
3.42E-07	4.05E-07	1.77E-11	4.05E-07	6.65E-11	7.47E-07	-6.126	5.73E 01
1.71E-07	2.87E-07	1.25E-11	2.87E-07	2.35E-11	4.58E-07	-6.339	7.02E 01
8.54E-08	2.03E-07	8.85E-12	2.03E-07	8.31E-12	2.88E-07	-6.540	8.84E 01
4.27E-08	1.43E-07	6.26E-12	1.43E-07	2.94E-12	1.86E-07	-6.730	1.14E 02
2.14E-08	1.01E-07	4.43E-12	1.01E-07	1.04E-12	1.23E-07	-6.911	1.51E 02
1.07E-08	7.17E-08	3.13E-12	7.17E-08	3.67E-13	8.24E-08	-7.084	2.02E 02
5.34E-09	5.07E-08	2.21E-12	5.07E-08	1.30E-13	5.60E-08	-7.252	2.75E 02
2.67E-09	3.58E-08	1.56E-12	3.58E-08	4.59E-14	3.85E-08	-7.414	3.78E 02
1.34E-09	2.53E-08	1.11E-12	2.53E-08	1.62E-14	2.67E-08	-7.574	5.23E 02
6.68E-10	1.79E-08	7.82E-13	1.79E-08	5.74E-15	1.86E-08	-7.731	7.29E 02
3.34E-10	1.27E-08	5.53E-13	1.27E-08	2.03E-15	1.30E-08	-7.886	1.02E 03
1.67E-10	8.96E-09	3.91E-13	8.96E-09	7.17E-16	9.13E-09	-8.040	1.43E 03
8.34E-11	6.34E-09	2.77E-13	6.34E-09	2.54E-16	6.42E-09	-8.193	2.02E 03
4.17E-11	4.48E-09	1.96E-13	4.48E-09	8.96E-17	4.52E-09	-8.345	2.84E 03
2.09E-11	3.17E-09	1.38E-13	3.17E-09	3.17E-17	3.19E-09	-8.496	4.00E 03
1.04E-11	2.24E-09	9.78E-14	2.24E-09	1.12E-17	2.25E-09	-8.648	5.65E 03
5.22E-12	1.58E-09	6.91E-14	1.58E-09	3.96E-18	1.59E-09	-8.799	7.98E 03
2.61E-12	1.12E-09	4.89E-14	1.12E-09	1.40E-18	1.12E-09	-8.950	1.13E 04
1.30E-12	7.92E-10	3.46E-14	7.92E-10	4.95E-19	7.93E-10	-9.101	1.59E 04

Table 10. Results of Calculations, t = 50°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 7.0
K1 = 2.62E 01 K2 = 4.80E 02 K3 = 4.80E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	5.62E-04	2.45E-10	2.40E-04	3.22E-04	3.68E-03	-2.434	3.45E 01
1.40E-03	3.36E-04	1.46E-10	2.01E-04	1.35E-04	1.87E-03	-2.728	3.50E 01
7.00E-04	2.12E-04	9.26E-11	1.59E-04	5.33E-05	9.65E-04	-3.015	3.61E 01
3.50E-04	1.40E-04	6.12E-11	1.20E-04	2.02E-05	5.10E-04	-3.292	3.82E 01
1.75E-04	9.56E-05	4.17E-11	8.82E-05	7.40E-06	2.78E-04	-3.556	4.16E 01
8.75E-05	6.62E-05	2.89E-11	6.36E-05	2.67E-06	1.56E-04	-3.806	4.68E 01
4.37E-05	4.64E-05	2.02E-11	4.54E-05	9.53E-07	9.11E-05	-4.041	5.45E 01
2.19E-05	3.26E-05	1.42E-11	3.23E-05	3.39E-07	5.48E-05	-4.261	6.57E 01
1.09E-05	2.30E-05	1.00E-11	2.29E-05	1.20E-07	3.41E-05	-4.468	8.16E 01
5.47E-06	1.62E-05	7.09E-12	1.62E-05	4.25E-08	2.18E-05	-4.662	1.04E 02
2.73E-06	1.15E-05	5.01E-12	1.15E-05	1.50E-08	1.42E-05	-4.847	1.36E 02
1.37E-06	8.12E-06	3.54E-12	8.11E-06	5.32E-09	9.49E-06	-5.023	1.82E 02
6.84E-07	5.74E-06	2.50E-12	5.74E-06	1.88E-09	6.42E-06	-5.192	2.46E 02
3.42E-07	4.06E-06	1.77E-12	4.06E-06	6.65E-10	4.40E-06	-5.357	3.37E 02
1.71E-07	2.87E-06	1.25E-12	2.87E-06	2.35E-10	3.04E-06	-5.517	4.66E 02
8.54E-08	2.03E-06	8.85E-13	2.03E-06	8.31E-11	2.11E-06	-5.675	6.48E 02
4.27E-08	1.43E-06	6.26E-13	1.43E-06	2.94E-11	1.48E-06	-5.831	9.06E 02
2.14E-08	1.01E-06	4.42E-13	1.01E-06	1.04E-11	1.04E-06	-5.985	1.27E 03
1.07E-08	7.17E-07	3.13E-13	7.17E-07	3.67E-12	7.28E-07	-6.138	1.79E 03
5.34E-09	5.07E-07	2.21E-13	5.07E-07	1.30E-12	5.12E-07	-6.290	2.51E 03
2.67E-09	3.59E-07	1.56E-13	3.59E-07	4.59E-13	3.61E-07	-6.442	3.54E 03
1.34E-09	2.54E-07	1.11E-13	2.54E-07	1.62E-13	2.55E-07	-6.594	5.00E 03
6.68E-10	1.79E-07	7.82E-14	1.79E-07	5.74E-14	1.80E-07	-6.745	7.06E 03
3.34E-10	1.27E-07	5.53E-14	1.27E-07	2.03E-14	1.27E-07	-6.896	9.98E 03
1.67E-10	8.96E-08	3.91E-14	8.96E-08	7.17E-15	8.98E-08	-7.047	1.41E 04
8.34E-11	6.34E-08	2.76E-14	6.34E-08	2.54E-15	6.35E-08	-7.197	1.99E 04
4.17E-11	4.48E-08	1.96E-14	4.48E-08	8.97E-16	4.49E-08	-7.348	2.82E 04
2.09E-11	3.17E-08	1.38E-14	3.17E-08	3.17E-16	3.17E-08	-7.499	3.98E 04
1.04E-11	2.24E-08	9.78E-15	2.24E-08	1.12E-16	2.24E-08	-7.649	5.63E 04
5.22E-12	1.58E-08	6.91E-15	1.58E-08	3.96E-17	1.59E-08	-7.800	7.96E 04
2.61E-12	1.12E-08	4.89E-15	1.12E-08	1.40E-17	1.12E-08	-7.951	1.13E 05
1.30E-12	7.92E-09	3.46E-15	7.92E-09	4.95E-18	7.92E-09	-8.101	1.59E 05
6.52E-13	5.60E-09	2.44E-15	5.60E-09	1.75E-18	5.60E-09	-8.252	2.25E 05
3.26E-13	3.96E-09	1.73E-15	3.96E-09	6.19E-19	3.96E-09	-8.402	3.18E 05
1.63E-13	2.80E-09	1.22E-15	2.80E-09	2.19E-19	2.80E-09	-8.553	4.50E 05
8.15E-14	1.98E-09	8.64E-16	1.98E-09	7.74E-20	1.98E-09	-8.703	6.37E 05
4.07E-14	1.40E-09	6.11E-16	1.40E-09	2.74E-20	1.40E-09	-8.854	9.01E 05
2.04E-14	9.90E-10	4.32E-16	9.90E-10	9.68E-21	9.90E-10	-9.004	1.27E 06

Table 11. Results of Calculations, t = 50°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 8.0
K1 = 2.62E 01 K2 = 4.80E 02 K3 = 4.80E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	1.78E-03	7.75E-11	7.59E-04	1.02E-03	5.60E-03	-2.252	5.24E 01
1.40E-03	1.06E-03	4.63E-11	6.35E-04	4.26E-04	2.89E-03	-2.539	5.40E 01
7.00E-04	6.71E-04	2.93E-11	5.02E-04	1.69E-04	1.54E-03	-2.813	5.76E 01
3.50E-04	4.44E-04	1.93E-11	3.80E-04	6.38E-05	8.57E-04	-3.067	6.42E 01
1.75E-04	3.02E-04	1.32E-11	2.79E-04	2.34E-05	5.01E-04	-3.300	7.50E 01
8.75E-05	2.10E-04	9.14E-12	2.01E-04	8.44E-06	3.05E-04	-3.515	9.15E 01
4.37E-05	1.47E-04	6.40E-12	1.44E-04	3.01E-06	1.93E-04	-3.713	1.16E 02
2.19E-05	1.03E-04	4.50E-12	1.02E-04	1.07E-06	1.26E-04	-3.899	1.51E 02
1.09E-05	7.28E-05	3.17E-12	7.24E-05	3.80E-07	8.41E-05	-4.075	2.01E 02
5.47E-06	5.14E-05	2.24E-12	5.13E-05	1.34E-07	5.70E-05	-4.244	2.73E 02
2.73E-06	3.63E-05	1.58E-12	3.63E-05	4.76E-08	3.91E-05	-4.408	3.75E 02
1.37E-06	2.57E-05	1.12E-12	2.57E-05	1.68E-08	2.71E-05	-4.568	5.18E 02
6.84E-07	1.81E-05	7.91E-13	1.81E-05	5.95E-09	1.88E-05	-4.725	7.22E 02
3.42E-07	1.28E-05	5.59E-13	1.28E-05	2.10E-09	1.32E-05	-4.880	1.01E 03
1.71E-07	9.07E-06	3.96E-13	9.07E-06	7.44E-10	9.24E-06	-5.034	1.42E 03
8.54E-08	6.42E-06	2.80E-13	6.41E-06	2.63E-10	6.50E-06	-5.187	1.99E 03
4.27E-08	4.54E-06	1.98E-13	4.54E-06	9.29E-11	4.58E-06	-5.339	2.81E 03
2.14E-08	3.21E-06	1.40E-13	3.21E-06	3.29E-11	3.23E-06	-5.491	3.96E 03
1.07E-08	2.27E-06	9.89E-14	2.27E-06	1.16E-11	2.28E-06	-5.642	5.59E 03
5.34E-09	1.60E-06	6.99E-14	1.60E-06	4.11E-12	1.61E-06	-5.793	7.89E 03
2.67E-09	1.13E-06	4.94E-14	1.13E-06	1.45E-12	1.14E-06	-5.944	1.12E 04
1.34E-09	8.02E-07	3.50E-14	8.02E-07	5.13E-13	8.03E-07	-6.095	1.58E 04
6.68E-10	5.67E-07	2.47E-14	5.67E-07	1.82E-13	5.68E-07	-6.246	2.23E 04
3.34E-10	4.01E-07	1.75E-14	4.01E-07	6.42E-14	4.01E-07	-6.397	3.15E 04
1.67E-10	2.84E-07	1.24E-14	2.84E-07	2.27E-14	2.84E-07	-6.547	4.45E 04
8.34E-11	2.00E-07	8.74E-15	2.00E-07	8.02E-15	2.01E-07	-6.698	6.30E 04
4.17E-11	1.42E-07	6.18E-15	1.42E-07	2.84E-15	1.42E-07	-6.848	8.90E 04
2.09E-11	1.00E-07	4.37E-15	1.00E-07	1.00E-15	1.00E-07	-6.999	1.26E 05
1.04E-11	7.09E-08	3.09E-15	7.09E-08	3.55E-16	7.09E-08	-7.149	1.78E 05
5.22E-12	5.01E-08	2.19E-15	5.01E-08	1.25E-16	5.01E-08	-7.300	2.52E 05
2.61E-12	3.54E-08	1.55E-15	3.54E-08	4.43E-17	3.54E-08	-7.450	3.56E 05
1.30E-12	2.51E-08	1.09E-15	2.51E-08	1.57E-17	2.51E-08	-7.601	5.04E 05
6.52E-13	1.77E-08	7.73E-16	1.77E-08	5.54E-18	1.77E-08	-7.752	7.12E 05
3.26E-13	1.25E-08	5.46E-16	1.25E-08	1.96E-18	1.25E-08	-7.902	1.01E 06
1.63E-13	8.86E-09	3.86E-16	8.86E-09	6.93E-19	8.86E-09	-8.053	1.42E 06
8.15E-14	6.26E-09	2.73E-16	6.26E-09	2.45E-19	6.26E-09	-8.203	2.01E 06
4.07E-14	4.43E-09	1.93E-16	4.43E-09	8.66E-20	4.43E-09	-8.354	2.85E 06
2.04E-14	3.13E-09	1.37E-16	3.13E-09	3.06E-20	3.13E-09	-8.504	4.03E 06
1.02E-14	2.21E-09	9.66E-17	2.21E-09	1.08E-20	2.21E-09	-8.655	5.70E 06
5.09E-15	1.57E-09	6.83E-17	1.57E-09	3.83E-21	1.57E-09	-8.805	8.06E 06

Table 12. Results of Calculations, t = 50°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 9.0
K1 = 2.62E-01 K2 = 4.80E-02 K3 = 4.80E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	5.62E-03	2.45E-11	2.40E-03	3.22E-03	1.16E-02	-1.934	1.09E 02
1.40E-03	3.36E-03	1.46E-11	2.01E-03	1.35E-03	6.11E-03	-2.214	1.14E 02
7.00E-04	2.12E-03	9.25E-12	1.59E-03	5.33E-04	3.36E-03	-2.474	1.26E 02
3.50E-04	1.40E-03	6.12E-12	1.20E-03	2.02E-04	1.96E-03	-2.709	1.46E 02
1.75E-04	9.56E-04	4.17E-12	8.82E-04	7.40E-05	1.21E-03	-2.919	1.80E 02
8.75E-05	6.63E-04	2.89E-12	6.36E-04	2.67E-05	7.77E-04	-3.110	2.33E 02
4.37E-05	4.64E-04	2.02E-12	4.54E-04	9.53E-06	5.17E-04	-3.286	3.10E 02
2.19E-05	3.26E-04	1.42E-12	3.23E-04	3.39E-06	3.52E-04	-3.454	4.21E 02
1.09E-05	2.30E-04	1.00E-12	2.29E-04	1.20E-06	2.42E-04	-3.616	5.80E 02
5.47E-06	1.63E-04	7.08E-13	1.62E-04	4.25E-07	1.68E-04	-3.774	8.07E 02
2.73E-06	1.15E-04	5.01E-13	1.15E-04	1.50E-07	1.18E-04	-3.929	1.13E 03
1.37E-06	8.12E-05	3.54E-13	8.11E-05	5.32E-08	8.26E-05	-4.083	1.58E 03
6.84E-07	5.74E-05	2.50E-13	5.74E-05	1.88E-08	5.81E-05	-4.236	2.23E 03
3.42E-07	4.06E-05	1.77E-13	4.06E-05	6.65E-09	4.09E-05	-4.388	3.14E 03
1.71E-07	2.87E-05	1.25E-13	2.87E-05	2.35E-09	2.89E-05	-4.540	4.43E 03
8.54E-08	2.03E-05	8.84E-14	2.03E-05	8.31E-10	2.04E-05	-4.691	6.25E 03
4.27E-08	1.43E-05	6.25E-14	1.43E-05	2.94E-10	1.44E-05	-4.842	8.82E 03
2.14E-08	1.01E-05	4.42E-14	1.01E-05	1.04E-10	1.02E-05	-4.993	1.25E 04
1.07E-08	7.17E-06	3.13E-14	7.17E-06	3.67E-11	7.18E-06	-5.144	1.76E 04
5.34E-09	5.07E-06	2.21E-14	5.07E-06	1.30E-11	5.08E-06	-5.294	2.49E 04
2.67E-09	3.59E-06	1.56E-14	3.59E-06	4.59E-12	3.59E-06	-5.445	3.52E 04
1.34E-09	2.54E-06	1.11E-14	2.54E-06	1.62E-12	2.54E-06	-5.596	4.98E 04
6.68E-10	1.79E-06	7.82E-15	1.79E-06	5.74E-13	1.79E-06	-5.746	7.04E 04
3.34E-10	1.27E-06	5.53E-15	1.27E-06	2.03E-13	1.27E-06	-5.897	9.96E 04
1.67E-10	8.97E-07	3.91E-15	8.97E-07	7.18E-14	8.97E-07	-6.047	1.41E 05
8.34E-11	6.34E-07	2.76E-15	6.34E-07	2.54E-14	6.34E-07	-6.198	1.99E 05
4.17E-11	4.48E-07	1.95E-15	4.48E-07	8.97E-15	4.48E-07	-6.348	2.82E 05
2.09E-11	3.17E-07	1.38E-15	3.17E-07	3.17E-15	3.17E-07	-6.499	3.98E 05
1.04E-11	2.24E-07	9.77E-16	2.24E-07	1.12E-15	2.24E-07	-6.649	5.63E 05
5.22E-12	1.59E-07	6.91E-16	1.59E-07	3.96E-16	1.59E-07	-6.800	7.96E 05
2.61E-12	1.12E-07	4.89E-16	1.12E-07	1.40E-16	1.12E-07	-6.950	1.13E 06
1.30E-12	7.93E-08	3.45E-16	7.93E-08	4.96E-17	7.93E-08	-7.101	1.59E 06
6.52E-13	5.60E-08	2.44E-16	5.60E-08	1.75E-17	5.60E-08	-7.251	2.25E 06
3.26E-13	3.96E-08	1.73E-16	3.96E-08	6.20E-18	3.96E-08	-7.402	3.19E 06
1.63E-13	2.80E-08	1.22E-16	2.80E-08	2.19E-18	2.80E-08	-7.552	4.50E 06
8.15E-14	1.98E-08	8.64E-17	1.98E-08	7.74E-19	1.98E-08	-7.703	6.37E 06
4.07E-14	1.40E-08	6.11E-17	1.40E-08	2.74E-19	1.40E-08	-7.854	9.01E 06
2.04E-14	9.91E-09	4.32E-17	9.91E-09	9.68E-20	9.91E-09	-8.004	1.27E 07
1.02E-14	7.01E-09	3.05E-17	7.01E-09	3.42E-20	7.01E-09	-8.155	1.80E 07
5.09E-15	4.95E-09	2.16E-17	4.95E-09	1.21E-20	4.95E-09	-8.305	2.55E 07

Table 13. Results of Calculations, t = 50°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 9.2
K1 = 2.62E-01 K2 = 4.80E-12 K3 = 4.90E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	7.[illegible]8E-03	1.95E-11	3.02E-03	4.06E-03	1.39E-02	-1.856	1.30E 02
1.40E-03	4.23E-03	1.16E-11	2.53E-03	1.70E-03	7.33E-03	-2.135	1.37E 02
7.00E-04	2.67E-03	7.35E-12	2.00E-03	6.72E-04	4.04E-03	-2.393	1.51E 02
3.50E-04	1.77E-03	4.86E-12	1.51E-03	2.54E-04	2.37E-03	-2.625	1.77E 02
1.75E-04	1.20E-03	3.31E-12	1.11E-03	9.32E-05	1.47E-03	-2.832	2.20E 02
8.75E-05	8.34E-04	2.29E-12	8.01E-04	3.36E-05	9.56E-04	-3.020	2.86E 02
4.37E-05	5.84E-04	1.61E-12	5.72E-04	1.20E-05	6.40E-04	-3.194	3.83E 02
2.19E-05	4.11E-04	1.13E-12	4.07E-04	4.27E-06	4.37E-04	-3.360	5.23E 02
1.09E-05	2.93E-04	7.97E-13	2.88E-04	1.51E-06	3.02E-04	-3.520	7.24E 02
5.47E-06	2.05E-04	5.63E-13	2.04E-04	5.35E-07	2.11E-04	-3.676	1.01E 03
2.73E-06	1.45E-04	3.98E-13	1.44E-04	1.89E-07	1.48E-04	-3.831	1.41E 03
1.37E-06	1.02E-04	2.81E-13	1.02E-04	6.70E-08	1.04E-04	-3.984	1.99E 03
6.84E-07	7.23E-05	1.99E-13	7.22E-05	2.37E-08	7.30E-05	-4.137	2.80E 03
3.42E-07	5.11E-05	1.41E-13	5.11E-05	8.37E-09	5.14E-05	-4.289	3.94E 03
1.71E-07	3.61E-05	9.93E-14	3.61E-05	2.96E-09	3.63E-05	-4.440	5.57E 03
8.54E-08	2.55E-05	7.02E-14	2.55E-05	1.05E-09	2.56E-05	-4.591	7.86E 03
4.27E-08	1.81E-05	4.97E-14	1.81E-05	3.70E-10	1.81E-05	-4.742	1.11E 04
2.14E-08	1.28E-05	3.51E-14	1.28E-05	1.31E-10	1.28E-05	-4.893	1.57E 04
1.07E-08	9.03E-06	2.48E-14	9.03E-06	4.63E-11	9.04E-06	-5.044	2.22E 04
5.34E-09	6.39E-06	1.76E-14	6.39E-06	1.64E-11	6.39E-06	-5.194	3.14E 04
2.67E-09	4.52E-06	1.24E-14	4.52E-06	5.78E-12	4.52E-06	-5.345	4.43E 04
1.34E-09	3.19E-06	8.78E-15	3.19E-06	2.04E-12	3.19E-06	-5.496	6.27E 04
6.68E-10	2.26E-06	6.21E-15	2.26E-06	7.23E-13	2.26E-06	-5.646	8.86E 04
3.34E-10	1.60E-06	4.39E-15	1.60E-06	2.56E-13	1.60E-06	-5.797	1.25E 05
1.67E-10	1.13E-06	3.10E-15	1.13E-06	9.04E-14	1.13E-06	-5.947	1.77E 05
8.34E-11	7.98E-07	2.20E-15	7.98E-07	3.19E-14	7.98E-07	-6.098	2.51E 05
4.17E-11	5.64E-07	1.55E-15	5.64E-07	1.13E-14	5.65E-07	-6.248	3.54E 05
2.09E-11	3.99E-07	1.10E-15	3.99E-07	3.99E-15	3.99E-07	-6.399	5.01E 05
1.04E-11	2.82E-07	7.76E-16	2.82E-07	1.41E-15	2.82E-07	-6.549	7.09E 05
5.22E-12	2.00E-07	5.49E-16	2.00E-07	4.99E-16	2.00E-07	-6.700	1.00E 06
2.61E-12	1.41E-07	3.88E-16	1.41E-07	1.76E-16	1.41E-07	-6.850	1.42E 06
1.30E-12	9.98E-08	2.74E-16	9.98E-08	6.24E-17	9.98E-08	-7.001	2.01E 06
6.52E-13	7.06E-08	1.94E-16	7.06E-08	2.21E-17	7.06E-08	-7.151	2.84E 06
3.26E-13	4.99E-08	1.37E-16	4.99E-08	7.80E-18	4.99E-08	-7.302	4.01E 06
1.63E-13	3.53E-08	9.70E-17	3.53E-08	2.76E-18	3.53E-08	-7.452	5.67E 06
8.15E-14	2.49E-08	6.86E-17	2.49E-08	9.75E-19	2.49E-08	-7.603	8.02E 06
4.07E-14	1.76E-08	4.85E-17	1.76E-08	3.45E-19	1.76E-08	-7.754	1.13E 07
2.04E-14	1.25E-08	3.43E-17	1.25E-08	1.22E-19	1.25E-08	-7.904	1.60E 07
1.02E-14	8.82E-09	2.43E-17	8.82E-09	4.31E-20	8.82E-09	-8.055	2.27E 07
5.09E-15	6.24E-09	1.72E-17	6.24E-09	1.52E-20	6.24E-09	-8.205	3.21E 07

Table 14. Results of Calculations, t = 50°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 50.0 DEG C PH = 9.5
K1 = 2.62E 01 K2 = 4.80E 02 K3 = 4.80E-12 K4 = 2.10E-11
SOLUBILITY OF I2 IN WATER = 2.80E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
2.80E-03	1.00E-02	1.38E-11	4.27E-03	5.73E-03	1.85E-02	-1.732	1.73E 02
1.40E-03	5.97E-03	8.23E-12	3.57E-03	2.40E-03	9.77E-03	-2.010	1.83E 02
7.00E-04	3.77E-03	5.20E-12	2.83E-03	9.49E-04	5.42E-03	-2.266	2.03E 02
3.50E-04	2.50E-03	3.44E-12	2.14E-03	3.59E-04	3.20E-03	-2.494	2.40E 02
1.75E-04	1.70E-03	2.34E-12	1.57E-03	1.32E-04	2.01E-03	-2.697	3.00E 02
8.75E-05	1.18E-03	1.62E-12	1.13E-03	4.75E-05	1.31E-03	-2.882	3.93E 02
4.37E-05	8.25E-04	1.14E-12	8.08E-04	1.70E-05	8.86E-04	-3.053	5.30E 02
2.19E-05	5.80E-04	8.00E-13	5.74E-04	6.03E-06	6.08E-04	-3.216	7.29E 02
1.09E-05	4.09E-04	5.64E-13	4.07E-04	2.14E-06	4.22E-04	-3.374	1.01E 03
5.47E-06	2.89E-04	3.98E-13	2.88E-04	7.56E-07	2.95E-04	-3.530	1.41E 03
2.73E-06	2.04E-04	2.81E-13	2.04E-04	2.68E-07	2.07E-04	-3.683	1.99E 03
1.37E-06	1.44E-04	1.99E-13	1.44E-04	9.46E-08	1.46E-04	-3.836	2.79E 03
6.84E-07	1.02E-04	1.41E-13	1.02E-04	3.35E-08	1.03E-04	-3.988	3.94E 03
3.42E-07	7.22E-05	9.95E-14	7.22E-05	1.18E-08	7.25E-05	-4.139	5.56E 03
1.71E-07	5.10E-05	7.03E-14	5.10E-05	4.18E-09	5.12E-05	-4.291	7.85E 03
8.54E-08	3.61E-05	4.97E-14	3.61E-05	1.48E-09	3.62E-05	-4.442	1.11E 04
4.27E-08	2.55E-05	3.52E-14	2.55E-05	5.23E-10	2.56E-05	-4.592	1.57E 04
2.14E-08	1.80E-05	2.49E-14	1.80E-05	1.85E-10	1.81E-05	-4.743	2.22E 04
1.07E-08	1.28E-05	1.76E-14	1.28E-05	6.54E-11	1.28E-05	-4.894	3.13E 04
5.34E-09	9.02E-06	1.24E-14	9.02E-06	2.31E-11	9.03E-06	-5.044	4.43E 04
2.67E-09	6.38E-06	8.79E-15	6.38E-06	8.17E-12	6.38E-06	-5.195	6.26E 04
1.34E-09	4.51E-06	6.22E-15	4.51E-06	2.89E-12	4.51E-06	-5.346	8.85E 04
6.68E-10	3.19E-06	4.40E-15	3.19E-06	1.02E-12	3.19E-06	-5.496	1.25E 05
3.34E-10	2.26E-06	3.11E-15	2.26E-06	3.61E-13	2.26E-06	-5.647	1.77E 05
1.67E-10	1.59E-06	2.20E-15	1.59E-06	1.28E-13	1.59E-06	-5.797	2.50E 05
8.34E-11	1.13E-06	1.55E-15	1.13E-06	4.51E-14	1.13E-06	-5.948	3.54E 05
4.17E-11	7.97E-07	1.10E-15	7.97E-07	1.60E-14	7.97E-07	-6.098	5.01E 05
2.09E-11	5.64E-07	7.77E-16	5.64E-07	5.64E-15	5.64E-07	-6.249	7.08E 05
1.04E-11	3.99E-07	5.49E-16	3.99E-07	1.99E-15	3.99E-07	-6.399	1.00E 06
5.22E-12	2.82E-07	3.88E-16	2.82E-07	7.05E-16	2.82E-07	-6.550	1.42E 06
2.61E-12	1.99E-07	2.75E-16	1.99E-07	2.49E-16	1.99E-07	-6.700	2.00E 06
1.30E-12	1.41E-07	1.94E-16	1.41E-07	8.81E-17	1.41E-07	-6.851	2.83E 06
6.52E-13	9.97E-08	1.37E-16	9.97E-08	3.12E-17	9.97E-08	-7.001	4.01E 06
3.26E-13	7.05E-08	9.71E-17	7.05E-08	1.10E-17	7.05E-08	-7.152	5.66E 06
1.63E-13	4.98E-08	6.87E-17	4.98E-08	3.90E-18	4.98E-08	-7.302	8.01E 06
8.15E-14	3.52E-08	4.86E-17	3.52E-08	1.38E-18	3.52E-08	-7.453	1.13E 07
4.07E-14	2.49E-08	3.43E-17	2.49E-08	4.87E-19	2.49E-08	-7.603	1.60E 07
2.04E-14	1.76E-08	2.43E-17	1.76E-08	1.72E-19	1.76E-08	-7.754	2.27E 07
1.02E-14	1.25E-08	1.72E-17	1.25E-08	6.09E-20	1.25E-08	-7.905	3.20E 07
5.09E-15	8.81E-09	1.21E-17	8.81E-09	2.15E-20	8.81E-09	-8.055	4.53E 07

Table 15. Results of Calculations, t = 80°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 5.0
K1 = 1.30E 01 K2 = 3.40E 12 K3 = 4.30E-11 K4 = 3.18E-11
SOLUBILITY OF I2 IN WATER = 8.86E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	3.92E-04	2.89E-09	9.75E-05	2.94E-04	9.55E-03	-2.020	1.40E 01
4.43E-03	2.19E-04	1.61E-09	3.72E-05	1.32E-04	4.78E-03	-2.321	1.40E 01
2.21E-03	1.29E-04	9.55E-10	7.38E-05	5.56E-05	2.40E-03	-2.620	1.41E 01
1.11E-03	8.11E-05	5.98E-10	5.89E-05	2.22E-05	1.21E-03	-2.917	1.42E 01
5.54E-04	5.33E-05	3.93E-10	4.48E-05	8.45E-06	6.15E-04	-3.211	1.44E 01
2.77E-04	3.61E-05	2.67E-10	3.30E-05	3.11E-06	3.16E-04	-3.500	1.48E 01
1.38E-04	2.50E-05	1.84E-10	2.39E-05	1.12E-06	1.65E-04	-3.784	1.55E 01
6.92E-05	1.75E-05	1.29E-10	1.71E-05	4.02E-07	8.71E-05	-4.060	1.64E 01
3.46E-05	1.23E-05	9.07E-11	1.21E-05	1.43E-07	4.70E-05	-4.328	1.77E 01
1.73E-05	8.66E-06	6.39E-11	8.61E-06	5.07E-08	2.60E-05	-4.585	1.95E 01
8.65E-06	6.11E-06	4.51E-11	6.10E-06	1.80E-08	1.48E-05	-4.830	2.22E 01
4.33E-06	4.32E-06	3.19E-11	4.31E-06	6.35E-09	8.65E-06	-5.063	2.60E 01
2.16E-06	3.05E-06	2.25E-11	3.05E-06	2.25E-09	5.22E-06	-5.282	3.14E 01
1.08E-06	2.16E-06	1.59E-11	2.16E-06	7.95E-10	3.24E-06	-5.489	3.90E 01
5.41E-07	1.53E-06	1.13E-11	1.53E-06	2.81E-10	2.07E-06	-5.685	4.97E 01
2.70E-07	1.08E-06	7.97E-12	1.08E-06	9.93E-11	1.35E-06	-5.870	6.49E 01
1.35E-07	7.63E-07	5.63E-12	7.63E-07	3.51E-11	8.98E-07	-6.046	8.64E 01
6.76E-08	5.40E-07	3.98E-12	5.40E-07	1.24E-11	6.07E-07	-6.217	1.17E 02
3.38E-08	3.82E-07	2.82E-12	3.82E-07	4.39E-12	4.15E-07	-6.382	1.60E 02
1.69E-08	2.70E-07	1.99E-12	2.70E-07	1.55E-12	2.87E-07	-6.543	2.21E 02
8.45E-09	1.91E-07	1.41E-12	1.91E-07	5.49E-13	1.99E-07	-6.701	3.07E 02
4.22E-09	1.35E-07	9.96E-13	1.35E-07	1.94E-13	1.39E-07	-6.857	4.28E 02
2.11E-09	9.54E-08	7.04E-13	9.54E-08	6.86E-14	9.75E-08	-7.011	6.00E 02
1.06E-09	6.75E-08	4.98E-13	6.75E-08	2.43E-14	6.85E-08	-7.164	8.43E 02
5.28E-10	4.77E-08	3.52E-13	4.77E-08	8.58E-15	4.82E-08	-7.317	1.19E 03
2.64E-10	3.37E-08	2.49E-13	3.37E-08	3.03E-15	3.40E-08	-7.469	1.67E 03
1.32E-10	2.39E-08	1.76E-13	2.39E-08	1.07E-15	2.40E-08	-7.620	2.36E 03
6.60E-11	1.69E-08	1.24E-13	1.69E-08	3.79E-16	1.69E-08	-7.771	3.33E 03
3.30E-11	1.19E-08	8.80E-14	1.19E-08	1.34E-16	1.20E-08	-7.922	4.71E 03
1.65E-11	8.43E-09	6.22E-14	8.43E-09	4.74E-17	8.45E-09	-8.073	6.66E 03
8.25E-12	5.96E-09	4.40E-14	5.96E-09	1.67E-17	5.97E-09	-8.224	9.41E 03
4.13E-12	4.22E-09	3.11E-14	4.22E-09	5.92E-18	4.22E-09	-8.375	1.33E 04
2.06E-12	2.98E-09	2.20E-14	2.98E-09	2.09E-18	2.98E-09	-8.525	1.88E 04
1.03E-12	2.11E-09	1.56E-14	2.11E-09	7.40E-19	2.11E-09	-8.676	2.66E 04
5.16E-13	1.49E-09	1.10E-14	1.49E-09	2.62E-19	1.49E-09	-8.826	3.76E 04
2.58E-13	1.05E-09	7.78E-15	1.05E-09	9.25E-20	1.05E-09	-8.977	5.32E 04
1.29E-13	7.45E-10	5.50E-15	7.45E-10	3.27E-20	7.45E-10	-9.128	7.52E 04

Table 16. Results of Calculations, t = 80°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 7.0
K1 = 1.30E-01 K2 = 3.40E-12 K3 = 4.30E-11 K4 = 3.18E-11
SOLUBILITY OF I2 IN WATER = 8.86E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	3.92E-03	2.89E-10	9.75E-04	2.94E-03	1.57E-02	-1.804	2.31E 01
4.43E-03	2.19E-03	1.61E-10	8.73E-04	1.32E-03	7.94E-03	-2.100	2.33E 01
2.21E-03	1.29E-03	9.54E-11	7.38E-04	5.56E-04	4.07E-03	-2.391	2.39E 01
1.11E-03	8.11E-04	5.98E-11	5.89E-04	2.22E-04	2.14E-03	-2.669	2.51E 01
5.54E-04	5.33E-04	3.93E-11	4.48E-04	8.45E-05	1.17E-03	-2.931	2.75E 01
2.77E-04	3.61E-04	2.67E-11	3.30E-04	3.11E-05	6.69E-04	-3.174	3.14E 01
1.38E-04	2.50E-04	1.84E-11	2.39E-04	1.13E-05	4.00E-04	-3.398	3.75E 01
6.92E-05	1.75E-04	1.29E-11	1.71E-04	4.02E-06	2.48E-04	-3.605	4.66E 01
3.46E-05	1.23E-04	9.06E-12	1.21E-04	1.43E-06	1.59E-04	-3.799	5.97E 01
1.73E-05	8.66E-05	6.39E-12	8.61E-05	5.07E-07	1.04E-04	-3.981	7.85E 01
8.65E-06	6.12E-05	4.51E-12	6.10E-05	1.80E-07	7.00E-05	-4.155	1.05E 02
4.33E-06	4.32E-05	3.19E-12	4.32E-05	6.36E-08	4.76E-05	-4.322	1.43E 02
2.16E-06	3.06E-05	2.25E-12	3.05E-05	2.25E-08	3.27E-05	-4.485	1.97E 02
1.08E-06	2.16E-05	1.59E-12	2.16E-05	7.95E-09	2.27E-05	-4.644	2.73E 02
5.41E-07	1.53E-05	1.13E-12	1.53E-05	2.81E-09	1.58E-05	-4.801	3.80E 02
2.70E-07	1.08E-05	7.96E-13	1.08E-05	9.94E-10	1.11E-05	-4.956	5.32E 02
1.35E-07	7.64E-06	5.63E-13	7.64E-06	3.51E-10	7.77E-06	-5.110	7.47E 02
6.76E-08	5.40E-06	3.98E-13	5.40E-06	1.24E-10	5.47E-06	-5.262	1.05E 03
3.38E-08	3.82E-06	2.82E-13	3.82E-06	4.39E-11	3.85E-06	-5.414	1.48E 03
1.69E-08	2.70E-06	1.99E-13	2.70E-06	1.55E-11	2.72E-06	-5.566	2.09E 03
8.45E-09	1.91E-06	1.41E-13	1.91E-06	5.49E-12	1.92E-06	-5.717	2.95E 03
4.22E-09	1.35E-06	9.95E-14	1.35E-06	1.94E-12	1.35E-06	-5.868	4.17E 03
2.11E-09	9.54E-07	7.04E-14	9.54E-07	6.86E-13	9.57E-07	-6.019	5.89E 03
1.06E-09	6.75E-07	4.98E-14	6.75E-07	2.43E-13	6.76E-07	-6.170	8.32E 03
5.28E-10	4.77E-07	3.52E-14	4.77E-07	8.58E-14	4.78E-07	-6.321	1.18E 04
2.64E-10	3.37E-07	2.49E-14	3.37E-07	3.03E-14	3.38E-07	-6.471	1.66E 04
1.32E-10	2.39E-07	1.76E-14	2.39E-07	1.07E-14	2.39E-07	-6.622	2.35E 04
6.60E-11	1.69E-07	1.24E-14	1.69E-07	3.79E-15	1.69E-07	-6.773	3.32E 04
3.30E-11	1.19E-07	8.80E-15	1.19E-07	1.34E-15	1.19E-07	-6.923	4.70E 04
1.65E-11	8.44E-08	6.22E-15	8.44E-08	4.74E-16	8.44E-08	-7.074	6.65E 04
8.25E-12	5.97E-08	4.40E-15	5.97E-08	1.68E-16	5.97E-08	-7.224	9.40E 04
4.13E-12	4.22E-08	3.11E-15	4.22E-08	5.92E-17	4.22E-08	-7.375	1.33E 05
2.06E-12	2.98E-08	2.20E-15	2.98E-08	2.09E-17	2.98E-08	-7.525	1.88E 05
1.03E-12	2.11E-08	1.56E-15	2.11E-08	7.40E-18	2.11E-08	-7.676	2.66E 05
5.16E-13	1.49E-08	1.10E-15	1.49E-08	2.62E-18	1.49E-08	-7.826	3.76E 05
2.58E-13	1.05E-08	7.78E-16	1.05E-08	9.26E-19	1.05E-08	-7.977	5.32E 05
1.29E-13	7.46E-09	5.50E-16	7.46E-09	3.27E-19	7.46E-09	-8.127	7.52E 05
6.45E-14	5.27E-09	3.89E-16	5.27E-09	1.16E-19	5.27E-09	-8.278	1.06E 06
3.22E-14	3.73E-09	2.75E-16	3.73E-09	4.09E-20	3.73E-09	-8.428	1.50E 06
1.61E-14	2.64E-09	1.94E-16	2.64E-09	1.45E-20	2.64E-09	-8.579	2.13E 06

Table 17. Results of Calculations, t = 80°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 8.0
K1 = 1.30E-01 K2 = 3.40E-02 K3 = 4.30E-11 K4 = 3.10E-11
SOLUBILITY OF I2 IN WATER = 8.86E-05 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	1.24E-02	9.13E-11	3.39E-03	9.30E-03	3.06E-02	-1.515	4.48E 01
4.43E-03	5.92E-03	5.17E-11	2.70E-03	4.16E-03	1.55E-02	-1.809	4.55E 01
2.21E-03	4.19E-03	3.32E-11	2.03E-03	1.70E-03	8.07E-03	-2.093	4.74E 01
1.11E-03	2.57E-03	1.69E-11	1.80E-03	7.02E-04	4.37E-03	-2.359	5.14E 01
5.54E-04	1.69E-03	1.24E-11	1.42E-03	2.67E-04	2.51E-03	-2.601	5.88E 01
2.77E-04	1.14E-03	5.43E-12	1.14E-03	9.85E-05	1.52E-03	-2.819	7.13E 01
1.38E-04	7.91E-04	5.83E-12	7.33E-04	3.56E-05	9.65E-04	-3.016	9.06E 01
6.92E-05	5.53E-04	4.03E-12	5.43E-04	1.27E-05	6.35E-04	-3.197	1.19E 02
3.46E-05	3.89E-04	2.86E-12	3.84E-04	4.53E-06	4.28E-04	-3.369	1.61E 02
1.73E-05	2.74E-04	2.02E-12	2.72E-04	1.60E-06	2.93E-04	-3.533	2.20E 02
8.65E-06	1.93E-04	1.43E-12	1.93E-04	5.68E-07	2.03E-04	-3.693	3.05E 02
4.33E-06	1.37E-04	1.01E-12	1.37E-04	2.01E-07	1.41E-04	-3.850	4.24E 02
2.16E-06	9.66E-05	7.12E-13	9.66E-05	7.11E-08	9.89E-05	-4.005	5.94E 02
1.08E-06	6.83E-05	5.04E-13	6.83E-05	2.51E-08	6.94E-05	-4.158	8.35E 02
5.41E-07	4.83E-05	3.56E-13	4.83E-05	8.89E-09	4.89E-05	-4.311	1.17E 03
2.70E-07	3.42E-05	2.52E-13	3.42E-05	3.14E-09	3.44E-05	-4.463	1.66E 03
1.35E-07	2.42E-05	1.78E-13	2.42E-05	1.11E-09	2.43E-05	-4.615	2.34E 03
6.76E-08	1.71E-05	1.26E-13	1.71E-05	3.93E-10	1.71E-05	-4.766	3.30E 03
3.38E-08	1.21E-05	8.93E-14	1.21E-05	1.39E-10	1.21E-05	-4.917	4.66E 03
1.69E-08	8.54E-06	6.29E-14	8.54E-06	4.91E-11	8.56E-06	-5.068	6.58E 03
8.45E-09	6.04E-06	4.45E-14	6.04E-06	1.74E-11	6.05E-06	-5.219	9.30E 03
4.22E-09	4.27E-06	3.15E-14	4.27E-06	6.14E-12	4.27E-06	-5.369	1.32E 04
2.11E-09	3.02E-06	2.23E-14	3.02E-06	2.17E-12	3.02E-06	-5.520	1.86E 04
1.06E-09	2.13E-06	1.57E-14	2.13E-06	7.67E-13	2.14E-06	-5.670	2.63E 04
5.28E-10	1.51E-06	1.11E-14	1.51E-06	2.71E-13	1.51E-06	-5.821	3.72E 04
2.64E-10	1.07E-06	7.87E-15	1.07E-06	9.59E-14	1.07E-06	-5.972	5.26E 04
1.32E-10	7.55E-07	5.56E-15	7.55E-07	3.39E-14	7.55E-07	-6.122	7.43E 04
6.60E-11	5.34E-07	3.93E-15	5.34E-07	1.20E-14	5.34E-07	-6.273	1.05E 05
3.30E-11	3.77E-07	2.78E-15	3.77E-07	4.24E-15	3.77E-07	-6.423	1.49E 05
1.65E-11	2.67E-07	1.97E-15	2.67E-07	1.50E-15	2.67E-07	-6.574	2.10E 05
8.25E-12	1.89E-07	1.39E-15	1.89E-07	5.30E-16	1.89E-07	-6.724	2.97E 05
4.13E-12	1.33E-07	9.83E-16	1.33E-07	1.87E-16	1.33E-07	-6.875	4.20E 05
2.06E-12	9.43E-08	6.95E-16	9.43E-08	6.62E-17	9.43E-08	-7.025	5.95E 05
1.03E-12	6.67E-08	4.92E-16	6.67E-08	2.34E-17	6.67E-08	-7.176	8.41E 05
5.16E-13	4.72E-08	3.48E-16	4.72E-08	8.28E-18	4.72E-08	-7.326	1.19E 06
2.58E-13	3.34E-08	2.46E-16	3.34E-08	2.93E-18	3.34E-08	-7.477	1.68E 06
1.29E-13	2.36E-08	1.74E-16	2.36E-08	1.04E-18	2.36E-08	-7.627	2.38E 06
6.45E-14	1.67E-08	1.23E-16	1.67E-08	3.66E-19	1.67E-08	-7.778	3.36E 06
3.22E-14	1.18E-08	8.69E-17	1.18E-08	1.29E-19	1.18E-08	-7.928	4.76E 06
1.61E-14	8.34E-09	6.15E-17	8.34E-09	4.57E-20	8.34E-09	-8.079	6.73E 06

IHCC021 STOP

Table 18. Results of Calculations, t = 80°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 9.0
K1 = 1.30E-01 K2 = 3.40E-02 K3 = 4.30E-11 K4 = 3.18E-11
SOLUBILITY OF I2 IN WATER = 8.86E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	3.92E-02	2.89E-11	9.76E-03	2.94E-02	7.75E-02	-1.111	1.14E 02
4.43E-03	2.19E-02	1.61E-11	3.73E-03	1.32E-02	3.95E-02	-1.403	1.16E 02
2.21E-03	1.29E-02	9.54E-12	7.38E-03	5.57E-03	2.07E-02	-1.683	1.22E 02
1.11E-03	8.11E-03	5.98E-12	5.89E-03	2.22E-03	1.14E-02	-1.942	1.34E 02
5.54E-04	5.33E-03	3.93E-12	4.48E-03	8.45E-04	6.73E-03	-2.172	1.58E 02
2.77E-04	3.62E-03	2.66E-12	3.30E-03	3.11E-04	4.20E-03	-2.376	1.97E 02
1.38E-04	2.50E-03	1.84E-12	2.39E-03	1.13E-04	2.75E-03	-2.560	2.58E 02
6.92E-05	1.75E-03	1.29E-12	1.71E-03	4.03E-05	1.86E-03	-2.731	3.49E 02
3.46E-05	1.23E-03	9.06E-13	1.22E-03	1.43E-05	1.28E-03	-2.893	4.80E 02
1.73E-05	8.67E-04	6.39E-13	8.62E-04	5.08E-06	8.89E-04	-3.051	6.68E 02
8.65E-06	6.12E-04	4.51E-13	6.10E-04	1.80E-06	6.22E-04	-3.206	9.35E 02
4.33E-06	4.32E-04	3.19E-13	4.32E-04	6.36E-07	4.37E-04	-3.359	1.31E 03
2.16E-06	3.06E-04	2.25E-13	3.05E-04	2.25E-07	3.08E-04	-3.511	1.85E 03
1.08E-06	2.16E-04	1.59E-13	2.16E-04	7.95E-08	2.17E-04	-3.663	2.61E 03
5.41E-07	1.53E-04	1.13E-13	1.53E-04	2.81E-08	1.53E-04	-3.814	3.69E 03
2.70E-07	1.08E-04	7.96E-14	1.08E-04	9.94E-09	1.08E-04	-3.965	5.21E 03
1.35E-07	7.64E-05	5.63E-14	7.64E-05	3.52E-09	7.65E-05	-4.116	7.36E 03
6.76E-08	5.40E-05	3.98E-14	5.40E-05	1.24E-09	5.41E-05	-4.267	1.04E 04
3.38E-08	3.82E-05	2.81E-14	3.82E-05	4.39E-10	3.82E-05	-4.418	1.47E 04
1.69E-08	2.70E-05	1.99E-14	2.70E-05	1.55E-10	2.70E-05	-4.568	2.08E 04
8.45E-09	1.91E-05	1.41E-14	1.91E-05	5.49E-11	1.91E-05	-4.719	2.94E 04
4.22E-09	1.35E-05	9.95E-15	1.35E-05	1.94E-11	1.35E-05	-4.869	4.16E 04
2.11E-09	9.55E-06	7.04E-15	9.55E-06	6.87E-12	9.55E-06	-5.020	5.88E 04
1.06E-09	6.75E-06	4.97E-15	6.75E-06	2.43E-12	6.75E-06	-5.171	8.31E 04
5.28E-10	4.77E-06	3.52E-15	4.77E-06	8.58E-13	4.77E-06	-5.321	1.18E 05
2.64E-10	3.38E-06	2.49E-15	3.38E-06	3.03E-13	3.38E-06	-5.472	1.66E 05
1.32E-10	2.39E-06	1.76E-15	2.39E-06	1.07E-13	2.39E-06	-5.622	2.35E 05
6.60E-11	1.69E-06	1.24E-15	1.69E-06	3.79E-14	1.69E-06	-5.773	3.32E 05
3.30E-11	1.19E-06	8.79E-16	1.19E-06	1.34E-14	1.19E-06	-5.923	4.70E 05
1.65E-11	8.44E-07	6.22E-16	8.44E-07	4.74E-15	8.44E-07	-6.074	6.65E 05
8.25E-12	5.97E-07	4.40E-16	5.97E-07	1.68E-15	5.97E-07	-6.224	9.40E 05
4.13E-12	4.22E-07	3.11E-16	4.22E-07	5.93E-16	4.22E-07	-6.375	1.33E 06
2.06E-12	2.98E-07	2.20E-16	2.98E-07	2.10E-16	2.98E-07	-6.525	1.88E 06
1.03E-12	2.11E-07	1.55E-16	2.11E-07	7.41E-17	2.11E-07	-6.676	2.66E 06
5.16E-13	1.49E-07	1.10E-16	1.49E-07	2.62E-17	1.49E-07	-6.826	3.76E 06
2.58E-13	1.05E-07	7.77E-17	1.05E-07	9.26E-18	1.05E-07	-6.977	5.32E 06
1.29E-13	7.46E-08	5.50E-17	7.46E-08	3.27E-18	7.46E-08	-7.127	7.52E 06
6.45E-14	5.27E-08	3.89E-17	5.27E-08	1.16E-18	5.27E-08	-7.278	1.06E 07
3.22E-14	3.73E-08	2.75E-17	3.73E-08	4.09E-19	3.73E-08	-7.428	1.50E 07
1.61E-14	2.64E-08	1.94E-17	2.64E-08	1.45E-19	2.64E-08	-7.579	2.13E 07

Table 19. Results of Calculations, t = 80°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 9.2
K1 = 1.30E-01 K2 = 3.40E-12 K3 = 4.30E-11 K4 = 3.18E-11
SOLUBILITY OF I2 IN WATER = 8.86E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	4.93E-02	2.29E-11	1.23E-02	3.71E-02	9.52E-02	-1.021	1.40E 02
4.43E-03	2.76E-02	1.28E-11	1.10E-02	1.66E-02	4.86E-02	-1.314	1.43E 02
2.21E-03	1.63E-02	7.58E-12	9.29E-03	7.01E-03	2.55E-02	-1.593	1.50E 02
1.11E-03	1.02E-02	4.75E-12	7.42E-03	2.80E-03	1.41E-02	-1.850	1.66E 02
5.54E-04	6.71E-03	3.12E-12	5.65E-03	1.06E-03	8.33E-03	-2.079	1.96E 02
2.77E-04	4.55E-03	2.12E-12	4.16E-03	3.92E-04	5.22E-03	-2.282	2.45E 02
1.38E-04	3.15E-03	1.46E-12	3.01E-03	1.42E-04	3.43E-03	-2.465	3.22E 02
6.92E-05	2.20E-03	1.02E-12	2.15E-03	5.07E-05	2.32E-03	-2.634	4.36E 02
3.46E-05	1.55E-03	7.19E-13	1.53E-03	1.80E-05	1.60E-03	-2.796	6.01E 02
1.73E-05	1.09E-03	5.07E-13	1.08E-03	6.39E-06	1.11E-03	-2.953	8.38E 02
8.65E-06	7.70E-04	3.58E-13	7.68E-04	2.26E-06	7.81E-04	-3.107	1.17E 03
4.33E-06	5.44E-04	2.53E-13	5.44E-04	8.01E-07	5.50E-04	-3.260	1.65E 03
2.16E-06	3.85E-04	1.79E-13	3.85E-04	2.83E-07	3.87E-04	-3.412	2.33E 03
1.08E-06	2.72E-04	1.26E-13	2.72E-04	1.00E-07	2.73E-04	-3.563	3.28E 03
5.41E-07	1.92E-04	8.94E-14	1.92E-04	3.54E-08	1.93E-04	-3.715	4.64E 03
2.70E-07	1.36E-04	6.32E-14	1.36E-04	1.25E-08	1.36E-04	-3.866	6.55E 03
1.35E-07	9.62E-05	4.47E-14	9.62E-05	4.43E-09	9.63E-05	-4.016	9.26E 03
6.76E-08	6.80E-05	3.16E-14	6.80E-05	1.56E-09	6.81E-05	-4.167	1.31E 04
3.38E-08	4.81E-05	2.24E-14	4.81E-05	5.53E-10	4.81E-05	-4.318	1.85E 04
1.69E-08	3.40E-05	1.58E-14	3.40E-05	1.96E-10	3.40E-05	-4.468	2.62E 04
8.45E-09	2.40E-05	1.12E-14	2.40E-05	6.92E-11	2.41E-05	-4.619	3.70E 04
4.22E-09	1.70E-05	7.90E-15	1.70E-05	2.44E-11	1.70E-05	-4.769	5.23E 04
2.11E-09	1.20E-05	5.59E-15	1.20E-05	8.64E-12	1.20E-05	-4.920	7.40E 04
1.06E-09	8.50E-06	3.95E-15	8.50E-06	3.06E-12	8.50E-06	-5.071	1.05E 05
5.28E-10	6.01E-06	2.79E-15	6.01E-06	1.08E-12	6.01E-06	-5.221	1.48E 05
2.64E-10	4.25E-06	1.98E-15	4.25E-06	3.82E-13	4.25E-06	-5.372	2.09E 05
1.32E-10	3.01E-06	1.40E-15	3.01E-06	1.35E-13	3.01E-06	-5.522	2.96E 05
6.60E-11	2.13E-06	9.88E-16	2.13E-06	4.78E-14	2.13E-06	-5.673	4.19E 05
3.30E-11	1.50E-06	6.98E-16	1.50E-06	1.69E-14	1.50E-06	-5.823	5.92E 05
1.65E-11	1.06E-06	4.94E-16	1.06E-06	5.97E-15	1.06E-06	-5.974	8.37E 05
8.25E-12	7.51E-07	3.49E-16	7.51E-07	2.11E-15	7.51E-07	-6.124	1.18E 06
4.13E-12	5.31E-07	2.47E-16	5.31E-07	7.46E-16	5.31E-07	-6.275	1.67E 06
2.06E-12	3.76E-07	1.75E-16	3.76E-07	2.64E-16	3.76E-07	-6.425	2.37E 06
1.03E-12	2.66E-07	1.23E-16	2.66E-07	9.33E-17	2.66E-07	-6.576	3.35E 06
5.16E-13	1.88E-07	8.73E-17	1.88E-07	3.30E-17	1.88E-07	-6.726	4.73E 06
2.58E-13	1.33E-07	6.17E-17	1.33E-07	1.17E-17	1.33E-07	-6.877	6.70E 06
1.29E-13	9.39E-08	4.37E-17	9.39E-08	4.12E-18	9.39E-08	-7.027	9.47E 06
6.45E-14	6.64E-08	3.09E-17	6.64E-08	1.46E-18	6.64E-08	-7.178	1.34E 07
3.22E-14	4.70E-08	2.18E-17	4.70E-08	5.15E-19	4.70E-08	-7.328	1.89E 07
1.61E-14	3.32E-08	1.54E-17	3.32E-08	1.82E-19	3.32E-08	-7.479	2.68E 07

Table 20. Results of Calculations, t = 80°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 80.0 DEG C PH = 9.5
K1 = 1.30E-01 K2 = 3.40E-02 K3 = 4.30E-11 K4 = 3.18E-11
SOLUBILITY OF I2 IN WATER = 8.86E-03 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
8.86E-03	6.97E-02	1.62E-11	1.74E-02	5.23E-02	1.31E-01	-0.883	1.92E 02
4.43E-03	3.89E-02	9.07E-12	1.55E-02	2.34E-02	6.68E-02	-1.175	1.96E 02
2.21E-03	2.30E-02	5.36E-12	1.31E-02	9.90E-03	3.51E-02	-1.454	2.06E 02
1.11E-03	1.44E-02	3.36E-12	1.05E-02	3.95E-03	1.95E-02	-1.710	2.29E 02
5.54E-04	9.48E-03	2.21E-12	7.98E-03	1.50E-03	1.15E-02	-1.938	2.71E 02
2.77E-04	6.43E-03	1.50E-12	5.88E-03	5.54E-04	7.26E-03	-2.139	3.41E 02
1.38E-04	4.45E-03	1.04E-12	4.25E-03	2.00E-04	4.79E-03	-2.320	4.50E 02
6.92E-05	3.11E-03	7.24E-13	3.04E-03	7.16E-05	3.25E-03	-2.488	6.11E 02
3.46E-05	2.19E-03	5.09E-13	2.16E-03	2.55E-05	2.25E-03	-2.649	8.44E 02
1.73E-05	1.54E-03	3.59E-13	1.53E-03	9.03E-06	1.57E-03	-2.805	1.18E 03
8.65E-06	1.09E-03	2.54E-13	1.09E-03	3.20E-06	1.10E-03	-2.959	1.65E 03
4.33E-06	7.69E-04	1.79E-13	7.68E-04	1.13E-06	7.75E-04	-3.111	2.33E 03
2.16E-06	5.44E-04	1.27E-13	5.43E-04	4.00E-07	5.46E-04	-3.263	3.28E 03
1.08E-06	3.84E-04	8.95E-14	3.84E-04	1.41E-07	3.86E-04	-3.414	4.63E 03
5.41E-07	2.72E-04	6.33E-14	2.72E-04	5.00E-08	2.72E-04	-3.565	6.55E 03
2.70E-07	1.92E-04	4.48E-14	1.92E-04	1.77E-08	1.92E-04	-3.716	9.25E 03
1.35E-07	1.36E-04	3.16E-14	1.36E-04	6.25E-09	1.36E-04	-3.866	1.31E 04
6.76E-08	9.61E-05	2.24E-14	9.61E-05	2.21E-09	9.61E-05	-4.017	1.85E 04
3.38E-08	6.79E-05	1.58E-14	6.79E-05	7.81E-10	6.80E-05	-4.168	2.61E 04
1.69E-08	4.80E-05	1.12E-14	4.80E-05	2.76E-10	4.80E-05	-4.318	3.70E 04
8.45E-09	3.40E-05	7.91E-15	3.40E-05	9.77E-11	3.40E-05	-4.469	5.23E 04
4.22E-09	2.40E-05	5.59E-15	2.40E-05	3.45E-11	2.40E-05	-4.619	7.39E 04
2.11E-09	1.70E-05	3.96E-15	1.70E-05	1.22E-11	1.70E-05	-4.770	1.05E 05
1.06E-09	1.20E-05	2.80E-15	1.20E-05	4.32E-12	1.20E-05	-4.921	1.48E 05
5.28E-10	8.49E-06	1.98E-15	8.49E-06	1.53E-12	8.49E-06	-5.071	2.09E 05
2.64E-10	6.00E-06	1.40E-15	6.00E-06	5.40E-13	6.00E-06	-5.222	2.96E 05
1.32E-10	4.25E-06	9.89E-16	4.25E-06	1.91E-13	4.25E-06	-5.372	4.18E 05
6.60E-11	3.00E-06	6.99E-16	3.00E-06	6.75E-14	3.00E-06	-5.523	5.91E 05
3.30E-11	2.12E-06	4.94E-16	2.12E-06	2.38E-14	2.12E-06	-5.673	8.36E 05
1.65E-11	1.50E-06	3.50E-16	1.50E-06	8.43E-15	1.50E-06	-5.824	1.18E 06
8.25E-12	1.06E-06	2.47E-16	1.06E-06	2.98E-15	1.06E-06	-5.974	1.67E 06
4.13E-12	7.50E-07	1.75E-16	7.50E-07	1.05E-15	7.50E-07	-6.125	2.36E 06
2.06E-12	5.31E-07	1.24E-16	5.31E-07	3.73E-16	5.31E-07	-6.275	3.34E 06
1.03E-12	3.75E-07	8.74E-17	3.75E-07	1.32E-16	3.75E-07	-6.426	4.73E 06
5.16E-13	2.65E-07	6.18E-17	2.65E-07	4.66E-17	2.65E-07	-6.576	6.69E 06
2.58E-13	1.88E-07	4.37E-17	1.88E-07	1.65E-17	1.88E-07	-6.727	9.46E 06
1.29E-13	1.33E-07	3.09E-17	1.33E-07	5.82E-18	1.33E-07	-6.877	1.34E 07
6.45E-14	9.38E-08	2.19E-17	9.38E-08	2.06E-18	9.38E-08	-7.028	1.89E 07
3.22E-14	6.63E-08	1.55E-17	6.63E-08	7.28E-19	6.63E-08	-7.178	2.68E 07
1.61E-14	4.69E-08	1.09E-17	4.69E-08	2.57E-19	4.69E-08	-7.329	3.78E 07

Table 21. Results of Calculations, t = 100°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 5.0
K1 = 9.00E-01 K2 = 2.98E-02 K3 = 1.50E-15 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	1.29E-03	3.32E-09	2.06E-04	1.07E-03	1.99E-02	-1.702	1.02E 01
8.75E-03	6.89E-04	1.79E-09	1.91E-04	4.98E-04	9.94E-03	-2.003	1.02E 01
4.37E-03	3.89E-04	1.01E-09	1.69E-04	2.20E-04	4.98E-03	-2.302	1.03E 01
2.19E-03	2.33E-04	6.05E-10	1.41E-04	9.19E-05	2.51E-03	-2.600	1.03E 01
1.09E-03	1.48E-04	3.83E-10	1.11E-04	3.63E-05	1.28E-03	-2.894	1.05E 01
5.47E-04	9.78E-05	2.54E-10	8.41E-05	1.37E-05	6.58E-04	-3.182	1.08E 01
2.73E-04	6.67E-05	1.73E-10	6.16E-05	5.02E-06	3.45E-04	-3.462	1.14E 01
1.37E-04	4.62E-05	1.20E-10	4.44E-05	1.81E-06	1.85E-04	-3.733	1.22E 01
6.84E-05	3.24E-05	8.40E-11	3.17E-05	6.46E-07	1.01E-04	-3.994	1.33E 01
3.42E-05	2.28E-05	5.91E-11	2.26E-05	2.30E-07	5.72E-05	-4.243	1.51E 01
1.71E-05	1.61E-05	4.17E-11	1.60E-05	8.14E-08	3.32E-05	-4.478	1.75E 01
8.54E-06	1.13E-05	2.94E-11	1.13E-05	2.88E-08	1.99E-05	-4.701	2.10E 01
4.27E-06	8.02E-06	2.08E-11	8.01E-06	1.02E-08	1.23E-05	-4.910	2.59E 01
2.14E-06	5.67E-06	1.47E-11	5.66E-06	3.60E-09	7.81E-06	-5.107	3.29E 01
1.07E-06	4.01E-06	1.04E-11	4.01E-06	1.27E-09	5.08E-06	-5.294	4.28E 01
5.34E-07	2.83E-06	7.35E-12	2.83E-06	4.51E-10	3.37E-06	-5.473	5.68E 01
2.67E-07	2.00E-06	5.20E-12	2.00E-06	1.59E-10	2.27E-06	-5.644	7.65E 01
1.34E-07	1.42E-06	3.68E-12	1.42E-06	5.63E-11	1.55E-06	-5.810	1.04E 02
6.68E-08	1.00E-06	2.60E-12	1.00E-06	1.99E-11	1.07E-06	-5.971	1.44E 02
3.34E-08	7.08E-07	1.84E-12	7.08E-07	7.04E-12	7.42E-07	-6.130	2.00E 02
1.67E-08	5.01E-07	1.30E-12	5.01E-07	2.49E-12	5.18E-07	-6.286	2.79E 02
8.34E-09	3.54E-07	9.19E-13	3.54E-07	8.80E-13	3.63E-07	-6.441	3.91E 02
4.17E-09	2.50E-07	6.50E-13	2.50E-07	3.11E-13	2.55E-07	-6.594	5.49E 02
2.09E-09	1.77E-07	4.59E-13	1.77E-07	1.10E-13	1.79E-07	-6.747	7.73E 02
1.04E-09	1.25E-07	3.25E-13	1.25E-07	3.89E-14	1.26E-07	-6.899	1.09E 03
5.22E-10	8.85E-08	2.30E-13	8.85E-08	1.38E-14	8.91E-08	-7.050	1.54E 03
2.61E-10	6.26E-08	1.62E-13	6.26E-08	4.86E-15	6.29E-08	-7.202	2.17E 03
1.30E-10	4.43E-08	1.15E-13	4.43E-08	1.72E-15	4.44E-08	-7.353	3.06E 03
6.52E-11	3.13E-08	8.12E-14	3.13E-08	6.08E-16	3.14E-08	-7.504	4.33E 03
3.26E-11	2.21E-08	5.74E-14	2.21E-08	2.15E-16	2.22E-08	-7.654	6.12E 03
1.63E-11	1.57E-08	4.06E-14	1.57E-08	7.60E-17	1.57E-08	-7.805	8.65E 03
8.15E-12	1.11E-08	2.87E-14	1.11E-08	2.69E-17	1.11E-08	-7.956	1.22E 04
4.07E-12	7.83E-09	2.03E-14	7.83E-09	9.50E-18	7.83E-09	-8.106	1.73E 04
2.04E-12	5.53E-09	1.44E-14	5.53E-09	3.36E-18	5.54E-09	-8.257	2.45E 04
1.02E-12	3.91E-09	1.02E-14	3.91E-09	1.19E-18	3.91E-09	-8.407	3.46E 04
5.09E-13	2.77E-09	7.18E-15	2.77E-09	4.20E-19	2.77E-09	-8.558	4.89E 04
2.55E-13	1.96E-09	5.08E-15	1.96E-09	1.48E-19	1.96E-09	-8.708	6.92E 04
1.27E-13	1.38E-09	3.59E-15	1.38E-09	5.25E-20	1.38E-09	-8.859	9.78E 04
6.37E-14	9.78E-10	2.54E-15	9.78E-10	1.85E-20	9.78E-10	-9.010	1.38E 05

Table 22. Results of Calculations, t = 100°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 7.0
K1 = 9.00E-00 K2 = 2.98E-02 K3 = 1.50E-10 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	1.28E-02	3.32E-10	2.06E-03	1.07E-02	4.10E-02	-1.387	2.11E 01
8.75E-03	6.89E-03	1.79E-10	1.91E-03	4.98E-03	2.06E-02	-1.686	2.12E 01
4.37E-03	3.89E-03	1.01E-10	1.69E-03	2.20E-03	1.05E-02	-1.980	2.15E 01
2.19E-03	2.33E-03	6.04E-11	1.41E-03	9.20E-04	5.44E-03	-2.265	2.24E 01
1.09E-03	1.48E-03	3.83E-11	1.11E-03	3.63E-04	2.93E-03	-2.533	2.41E 01
5.47E-04	9.78E-04	2.54E-11	8.41E-04	1.37E-04	1.66E-03	-2.779	2.74E 01
2.73E-04	6.67E-04	1.73E-11	6.17E-04	5.02E-05	9.91E-04	-3.004	3.26E 01
1.37E-04	4.63E-04	1.20E-11	4.45E-04	1.81E-05	6.17E-04	-3.209	4.06E 01
6.84E-05	3.24E-04	8.40E-12	3.17E-04	6.46E-06	3.99E-04	-3.399	5.25E 01
3.42E-05	2.28E-04	5.91E-12	2.26E-04	2.30E-06	2.64E-04	-3.578	6.96E 01
1.71E-05	1.61E-04	4.17E-12	1.60E-04	8.14E-07	1.79E-04	-3.748	9.41E 01
8.54E-06	1.14E-04	2.94E-12	1.13E-04	2.88E-07	1.22E-04	-3.912	1.29E 02
4.27E-06	8.02E-05	2.08E-12	8.01E-05	1.02E-07	8.46E-05	-4.073	1.78E 02
2.14E-06	5.67E-05	1.47E-12	5.67E-05	3.61E-08	5.89E-05	-4.230	2.48E 02
1.07E-06	4.01E-05	1.04E-12	4.01E-05	1.27E-08	4.12E-05	-4.385	3.47E 02
5.34E-07	2.83E-05	7.35E-13	2.83E-05	4.51E-09	2.89E-05	-4.539	4.87E 02
2.67E-07	2.00E-05	5.20E-13	2.00E-05	1.59E-09	2.03E-05	-4.692	6.85E 02
1.34E-07	1.42E-05	3.67E-13	1.42E-05	5.63E-10	1.43E-05	-4.844	9.64E 02
6.68E-08	1.00E-05	2.60E-13	1.00E-05	1.99E-10	1.01E-05	-4.996	1.36E 03
3.34E-08	7.09E-06	1.84E-13	7.09E-06	7.04E-11	7.12E-06	-5.148	1.92E 03
1.67E-08	5.01E-06	1.30E-13	5.01E-06	2.49E-11	5.03E-06	-5.299	2.71E 03
8.34E-09	3.54E-06	9.19E-14	3.54E-06	8.80E-12	3.55E-06	-5.450	3.83E 03
4.17E-09	2.51E-06	6.50E-14	2.51E-06	3.11E-12	2.51E-06	-5.600	5.41E 03
2.09E-09	1.77E-06	4.59E-14	1.77E-06	1.10E-12	1.77E-06	-5.751	7.65E 03
1.04E-09	1.25E-06	3.25E-14	1.25E-06	3.89E-13	1.25E-06	-5.902	1.08E 04
5.22E-10	8.86E-07	2.30E-14	8.86E-07	1.38E-13	8.86E-07	-6.052	1.53E 04
2.61E-10	6.26E-07	1.62E-14	6.26E-07	4.86E-14	6.27E-07	-6.203	2.16E 04
1.30E-10	4.43E-07	1.15E-14	4.43E-07	1.72E-14	4.43E-07	-6.354	3.06E 04
6.52E-11	3.13E-07	8.12E-15	3.13E-07	6.08E-15	3.13E-07	-6.504	4.32E 04
3.26E-11	2.21E-07	5.74E-15	2.21E-07	2.15E-15	2.21E-07	-6.655	6.11E 04
1.63E-11	1.57E-07	4.06E-15	1.57E-07	7.60E-16	1.57E-07	-6.805	8.65E 04
8.15E-12	1.11E-07	2.87E-15	1.11E-07	2.69E-16	1.11E-07	-6.956	1.22E 05
4.07E-12	7.83E-08	2.03E-15	7.83E-08	9.50E-17	7.83E-08	-7.106	1.73E 05
2.04E-12	5.54E-08	1.44E-15	5.54E-08	3.36E-17	5.54E-08	-7.257	2.45E 05
1.02E-12	3.91E-08	1.01E-15	3.91E-08	1.19E-17	3.91E-08	-7.407	3.46E 05
5.09E-13	2.77E-08	7.18E-16	2.77E-08	4.20E-18	2.77E-08	-7.558	4.89E 05
2.55E-13	1.96E-08	5.07E-16	1.96E-08	1.48E-18	1.96E-08	-7.708	6.92E 05
1.27E-13	1.38E-08	3.59E-16	1.38E-08	5.25E-19	1.38E-08	-7.859	9.78E 05
6.37E-14	9.79E-09	2.54E-16	9.79E-09	1.86E-19	9.79E-09	-8.009	1.38E 06
3.18E-14	6.92E-09	1.79E-16	6.92E-09	6.56E-20	6.92E-09	-8.160	1.96E 06

Table 23. Results of Calculations, t = 100°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 8.0
K1 = 9.00E-02 K2 = 2.98E-02 K3 = 1.50E-10 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	4.24E-02	1.05E-10	6.51E-03	3.39E-02	9.19E-02	-1.037	4.73E 01
8.75E-03	2.18E-02	5.65E-11	6.04E-03	1.57E-02	4.63E-02	-1.335	4.76E 01
4.37E-03	1.23E-02	3.19E-11	5.35E-03	6.97E-03	2.37E-02	-1.626	4.87E 01
2.19E-03	7.37E-03	1.91E-11	4.46E-03	2.91E-03	1.25E-02	-1.904	5.13E 01
1.09E-03	4.67E-03	1.21E-11	3.52E-03	1.15E-03	6.91E-03	-2.160	5.69E 01
5.47E-04	3.09E-03	8.02E-12	2.66E-03	4.33E-04	4.07E-03	-2.390	6.70E 01
2.73E-04	2.11E-03	5.47E-12	1.95E-03	1.59E-04	2.54E-03	-2.595	8.37E 01
1.37E-04	1.46E-03	3.79E-12	1.41E-03	5.72E-05	1.66E-03	-2.781	1.09E 02
6.84E-05	1.02E-03	2.66E-12	1.00E-03	2.04E-05	1.11E-03	-2.953	1.47E 02
3.42E-05	7.21E-04	1.87E-12	7.14E-04	7.26E-06	7.62E-04	-3.118	2.01E 02
1.71E-05	5.08E-04	1.32E-12	5.06E-04	2.57E-06	5.28E-04	-3.277	2.78E 02
8.54E-06	3.59E-04	9.30E-13	3.58E-04	9.11E-07	3.69E-04	-3.434	3.88E 02
4.27E-06	2.54E-04	6.58E-13	2.53E-04	3.22E-07	2.58E-04	-3.588	5.44E 02
2.14E-06	1.79E-04	4.65E-13	1.79E-04	1.14E-07	1.82E-04	-3.741	7.65E 02
1.07E-06	1.27E-04	3.29E-13	1.27E-04	4.03E-08	1.28E-04	-3.893	1.08E 03
5.34E-07	8.97E-05	2.32E-13	8.96E-05	1.43E-08	9.02E-05	-4.045	1.52E 03
2.67E-07	6.34E-05	1.64E-13	6.34E-05	5.04E-09	6.37E-05	-4.196	2.15E 03
1.34E-07	4.48E-05	1.16E-13	4.48E-05	1.78E-09	4.50E-05	-4.347	3.03E 03
6.68E-08	3.17E-05	8.21E-14	3.17E-05	6.30E-10	3.18E-05	-4.498	4.28E 03
3.34E-08	2.24E-05	5.81E-14	2.24E-05	2.23E-10	2.24E-05	-4.649	6.05E 03
1.67E-08	1.58E-05	4.11E-14	1.58E-05	7.88E-11	1.59E-05	-4.800	8.56E 03
8.34E-09	1.12E-05	2.90E-14	1.12E-05	2.78E-11	1.12E-05	-4.950	1.21E 04
4.17E-09	7.92E-06	2.05E-14	7.92E-06	9.85E-12	7.93E-06	-5.101	1.71E 04
2.09E-09	5.60E-06	1.45E-14	5.60E-06	3.48E-12	5.61E-06	-5.251	2.42E 04
1.04E-09	3.96E-06	1.03E-14	3.96E-06	1.23E-12	3.96E-06	-5.402	3.42E 04
5.22E-10	2.80E-06	7.26E-15	2.80E-06	4.35E-13	2.80E-06	-5.553	4.84E 04
2.61E-10	1.98E-06	5.13E-15	1.98E-06	1.54E-13	1.98E-06	-5.703	6.84E 04
1.30E-10	1.40E-06	3.63E-15	1.40E-06	5.44E-14	1.40E-06	-5.854	9.67E 04
6.52E-11	9.91E-07	2.57E-15	9.91E-07	1.92E-14	9.91E-07	-6.004	1.37E 05
3.26E-11	7.00E-07	1.82E-15	7.00E-07	6.80E-15	7.00E-07	-6.155	1.93E 05
1.63E-11	4.95E-07	1.28E-15	4.95E-07	2.40E-15	4.95E-07	-6.305	2.73E 05
8.15E-12	3.50E-07	9.08E-16	3.50E-07	8.50E-16	3.50E-07	-6.456	3.87E 05
4.07E-12	2.48E-07	6.42E-16	2.48E-07	3.00E-16	2.48E-07	-6.606	5.47E 05
2.04E-12	1.75E-07	4.54E-16	1.75E-07	1.06E-16	1.75E-07	-6.757	7.74E 05
1.02E-12	1.24E-07	3.21E-16	1.24E-07	3.76E-17	1.24E-07	-6.907	1.09E 06
5.09E-13	8.76E-08	2.27E-16	8.76E-08	1.33E-17	8.76E-08	-7.058	1.55E 06
2.55E-13	6.19E-08	1.60E-16	6.19E-08	4.69E-18	6.19E-08	-7.208	2.19E 06
1.27E-13	4.38E-08	1.13E-16	4.38E-08	1.66E-18	4.38E-08	-7.359	3.09E 06
6.37E-14	3.10E-08	8.02E-17	3.10E-08	5.87E-19	3.10E-08	-7.509	4.38E 06
3.18E-14	2.19E-08	5.67E-17	2.19E-08	2.07E-19	2.19E-08	-7.660	6.19E 06

Table 24. Results of Calculations, t = 100°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 9.0
K1 = 9.00E-02 K2 = 2.98E-02 K3 = 1.50E-10 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	1.28E-01	3.31E-11	2.06E-02	1.07E-01	2.53E-01	-0.597	1.30E 02
8.75E-03	6.89E-02	1.79E-11	1.91E-02	4.98E-02	1.27E-01	-0.895	1.31E 02
4.37E-03	3.89E-02	1.01E-11	1.69E-02	2.20E-02	6.54E-02	-1.185	1.34E 02
2.19E-03	2.33E-02	6.04E-12	1.41E-02	9.20E-03	3.47E-02	-1.460	1.43E 02
1.09E-03	1.48E-02	3.83E-12	1.11E-02	3.63E-03	1.95E-02	-1.710	1.60E 02
5.47E-04	9.73E-03	2.53E-12	8.41E-03	1.37E-03	1.17E-02	-1.932	1.93E 02
2.73E-04	6.67E-03	1.73E-12	6.17E-03	5.02E-04	7.45E-03	-2.128	2.45E 02
1.37E-04	4.63E-03	1.20E-12	4.45E-03	1.81E-04	4.95E-03	-2.306	3.26E 02
6.84E-05	3.24E-03	8.39E-13	3.18E-03	6.47E-05	3.37E-03	-2.472	4.44E 02
3.42E-05	2.28E-03	5.91E-13	2.26E-03	2.30E-05	2.34E-03	-2.631	6.15E 02
1.71E-05	1.61E-03	4.17E-13	1.60E-03	8.14E-06	1.63E-03	-2.787	8.60E 02
8.54E-06	1.14E-03	2.94E-13	1.13E-03	2.88E-06	1.15E-03	-2.940	1.21E 03
4.27E-06	8.08E-04	2.08E-13	8.02E-04	1.02E-06	8.08E-04	-3.093	1.70E 03
2.14E-06	5.67E-04	1.47E-13	5.67E-04	3.61E-07	5.70E-04	-3.244	2.40E 03
1.07E-06	4.01E-04	1.04E-13	4.01E-04	1.28E-07	4.02E-04	-3.395	3.39E 03
5.34E-07	2.84E-04	7.35E-14	2.84E-04	4.51E-08	2.84E-04	-3.546	4.79E 03
2.67E-07	2.01E-04	5.19E-14	2.01E-04	1.59E-08	2.01E-04	-3.697	6.77E 03
1.34E-07	1.42E-04	3.67E-14	1.42E-04	5.64E-09	1.42E-04	-3.848	9.57E 03
6.68E-08	1.00E-04	2.60E-14	1.00E-04	1.99E-09	1.00E-04	-3.999	1.35E 04
3.34E-08	7.09E-05	1.84E-14	7.09E-05	7.05E-10	7.09E-05	-4.149	1.91E 04
1.67E-08	5.01E-05	1.30E-14	5.01E-05	2.49E-10	5.01E-05	-4.300	2.70E 04
8.34E-09	3.54E-05	9.18E-15	3.54E-05	8.81E-11	3.55E-05	-4.450	3.82E 04
4.17E-09	2.51E-05	6.49E-15	2.51E-05	3.11E-11	2.51E-05	-4.601	5.41E 04
2.09E-09	1.77E-05	4.59E-15	1.77E-05	1.10E-11	1.77E-05	-4.751	7.65E 04
1.04E-09	1.25E-05	3.25E-15	1.25E-05	3.89E-12	1.25E-05	-4.902	1.08E 05
5.22E-10	8.86E-06	2.30E-15	8.86E-06	1.38E-12	8.86E-06	-5.052	1.53E 05
2.61E-10	6.27E-06	1.62E-15	6.27E-06	4.87E-13	6.27E-06	-5.203	2.16E 05
1.30E-10	4.43E-06	1.15E-15	4.43E-06	1.72E-13	4.43E-06	-5.354	3.06E 05
6.52E-11	3.13E-06	8.12E-16	3.13E-06	6.08E-14	3.13E-06	-5.504	4.33E 05
3.26E-11	2.22E-06	5.74E-16	2.22E-06	2.15E-14	2.22E-06	-5.655	6.12E 05
1.63E-11	1.57E-06	4.06E-16	1.57E-06	7.60E-15	1.57E-06	-5.805	8.65E 05
8.15E-12	1.11E-06	2.87E-16	1.11E-06	2.69E-15	1.11E-06	-5.956	1.22E 06
4.07E-12	7.83E-07	2.03E-16	7.83E-07	9.50E-16	7.83E-07	-6.106	1.73E 06
2.04E-12	5.54E-07	1.43E-16	5.54E-07	3.36E-16	5.54E-07	-6.257	2.45E 06
1.02E-12	3.92E-07	1.01E-16	3.92E-07	1.19E-16	3.92E-07	-6.407	3.46E 06
5.09E-13	2.77E-07	7.17E-17	2.77E-07	4.20E-17	2.77E-07	-6.558	4.89E 06
2.55E-13	1.96E-07	5.07E-17	1.96E-07	1.48E-17	1.96E-07	-6.708	6.92E 06
1.27E-13	1.38E-07	3.59E-17	1.38E-07	5.25E-18	1.38E-07	-6.859	9.79E 06
6.37E-14	9.79E-08	2.54E-17	9.79E-08	1.86E-18	9.79E-08	-7.009	1.38E 07
3.18E-14	6.92E-08	1.79E-17	6.92E-08	6.56E-19	6.92E-08	-7.160	1.96E 07

Table 25. Results of Calculations, t = 100°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 9.2
K1 = 9.00E-03 K2 = 2.98E-02 K3 = 1.50E-10 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	1.61E-01	2.63E-11	2.59E-02	1.35E-01	3.14E-01	-0.504	1.61E 02
8.75E-03	8.68E-02	1.42E-11	2.41E-02	6.27E-02	1.58E-01	-0.801	1.63E 02
4.37E-03	4.90E-02	8.01E-12	2.13E-02	2.77E-02	8.11E-02	-1.091	1.67E 02
2.19E-03	2.94E-02	4.80E-12	1.78E-02	1.16E-02	4.31E-02	-1.365	1.77E 02
1.09E-03	1.86E-02	3.04E-12	1.40E-02	4.57E-03	2.43E-02	-1.615	2.00E 02
5.47E-04	1.23E-02	2.01E-12	1.06E-02	1.73E-03	1.46E-02	-1.836	2.40E 02
2.73E-04	8.40E-03	1.37E-12	7.77E-03	6.33E-04	9.31E-03	-2.031	3.06E 02
1.37E-04	5.83E-03	9.52E-13	5.60E-03	2.28E-04	6.19E-03	-2.208	4.08E 02
6.84E-05	4.08E-03	6.67E-13	4.00E-03	8.14E-05	4.23E-03	-2.374	5.57E 02
3.42E-05	2.87E-03	4.69E-13	2.84E-03	2.89E-05	2.93E-03	-2.533	7.72E 02
1.71E-05	2.02E-03	3.31E-13	2.01E-03	1.03E-05	2.05E-03	-2.688	1.08E 03
8.54E-06	1.43E-03	2.34E-13	1.43E-03	3.63E-06	1.44E-03	-2.841	1.52E 03
4.27E-06	1.01E-03	1.65E-13	1.01E-03	1.28E-06	1.02E-03	-2.993	2.14E 03
2.14E-06	7.14E-04	1.17E-13	7.14E-04	4.54E-07	7.17E-04	-3.145	3.02E 03
1.07E-06	5.05E-04	8.25E-14	5.05E-04	1.61E-07	5.06E-04	-3.296	4.27E 03
5.34E-07	3.57E-04	5.83E-14	3.57E-04	5.68E-08	3.58E-04	-3.447	6.03E 03
2.67E-07	2.52E-04	4.13E-14	2.52E-04	2.01E-08	2.53E-04	-3.597	8.52E 03
1.34E-07	1.79E-04	2.92E-14	1.78E-04	7.10E-09	1.79E-04	-3.748	1.20E 04
6.68E-08	1.26E-04	2.06E-14	1.26E-04	2.51E-09	1.26E-04	-3.899	1.70E 04
3.34E-08	8.93E-05	1.46E-14	8.92E-05	8.87E-10	8.93E-05	-4.049	2.41E 04
1.67E-08	6.31E-05	1.03E-14	6.31E-05	3.14E-10	6.31E-05	-4.200	3.40E 04
8.34E-09	4.46E-05	7.29E-15	4.46E-05	1.11E-10	4.46E-05	-4.350	4.81E 04
4.17E-09	3.16E-05	5.16E-15	3.16E-05	3.92E-11	3.16E-05	-4.501	6.81E 04
2.09E-09	2.23E-05	3.65E-15	2.23E-05	1.39E-11	2.23E-05	-4.651	9.63E 04
1.04E-09	1.58E-05	2.58E-15	1.58E-05	4.90E-12	1.58E-05	-4.802	1.36E 05
5.22E-10	1.12E-05	1.82E-15	1.12E-05	1.73E-12	1.12E-05	-4.952	1.93E 05
2.61E-10	7.89E-06	1.29E-15	7.89E-06	6.13E-13	7.89E-06	-5.103	2.72E 05
1.30E-10	5.58E-06	9.12E-16	5.58E-06	2.17E-13	5.58E-06	-5.254	3.85E 05
6.52E-11	3.94E-06	6.45E-16	3.94E-06	7.66E-14	3.94E-06	-5.404	5.45E 05
3.26E-11	2.79E-06	4.56E-16	2.79E-06	2.71E-14	2.79E-06	-5.555	7.70E 05
1.63E-11	1.97E-06	3.22E-16	1.97E-06	9.57E-15	1.97E-06	-5.705	1.09E 06
8.15E-12	1.39E-06	2.28E-16	1.39E-06	3.38E-15	1.39E-06	-5.856	1.54E 06
4.07E-12	9.86E-07	1.61E-16	9.86E-07	1.20E-15	9.86E-07	-6.006	2.18E 06
2.04E-12	6.97E-07	1.14E-16	6.97E-07	4.23E-16	6.97E-07	-6.157	3.08E 06
1.02E-12	4.93E-07	8.06E-17	4.93E-07	1.50E-16	4.93E-07	-6.307	4.36E 06
5.09E-13	3.49E-07	5.70E-17	3.49E-07	5.29E-17	3.49E-07	-6.458	6.16E 06
2.55E-13	2.47E-07	4.03E-17	2.47E-07	1.87E-17	2.47E-07	-6.608	8.71E 06
1.27E-13	1.74E-07	2.85E-17	1.74E-07	6.61E-18	1.74E-07	-6.759	1.23E 07
6.37E-14	1.23E-07	2.01E-17	1.23E-07	2.34E-18	1.23E-07	-6.909	1.74E 07
3.18E-14	8.72E-08	1.42E-17	8.72E-08	8.26E-19	8.72E-08	-7.060	2.46E 07

Table 26. Results of Calculations, t = 100°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 100.0 DEG C PH = 9.5
K1 = 9.00E 00 K2 = 2.98E 02 K3 = 1.50E-10 K4 = 3.90E-11
SOLUBILITY OF I2 IN WATER = 1.75E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
1.75E-02	2.28E-01	1.86E-11	3.66E-02	1.91E-01	4.36E-01	-0.361	2.24E 02
8.75E-03	1.23E-01	1.00E-11	3.40E-02	8.86E-02	2.20E-01	-0.658	2.26E 02
4.37E-03	6.93E-02	5.67E-12	3.01E-02	3.92E-02	1.13E-01	-0.948	2.32E 02
2.19E-03	4.15E-02	3.40E-12	2.51E-02	1.64E-02	6.00E-02	-1.222	2.47E 02
1.09E-03	2.63E-02	2.15E-12	1.98E-02	6.46E-03	3.38E-02	-1.471	2.78E 02
5.47E-04	1.74E-02	1.43E-12	1.50E-02	2.44E-03	2.04E-02	-1.691	3.36E 02
2.73E-04	1.19E-02	9.72E-13	1.10E-02	8.94E-04	1.30E-02	-1.885	4.29E 02
1.37E-04	8.23E-03	6.74E-13	7.91E-03	3.22E-04	8.69E-03	-2.061	5.72E 02
6.84E-05	5.76E-03	4.72E-13	5.65E-03	1.15E-04	5.95E-03	-2.226	7.83E 02
3.42E-05	4.05E-03	3.32E-13	4.01E-03	4.09E-05	4.13E-03	-2.384	1.09E 03
1.71E-05	2.86E-03	2.34E-13	2.85E-03	1.45E-05	2.89E-03	-2.539	1.52E 03
8.54E-06	2.02E-03	1.65E-13	2.01E-03	5.13E-06	2.03E-03	-2.692	2.14E 03
4.27E-06	1.43E-03	1.17E-13	1.43E-03	1.81E-06	1.43E-03	-2.844	3.02E 03
2.14E-06	1.01E-03	8.26E-14	1.01E-03	6.41E-07	1.01E-03	-2.995	4.26E 03
1.07E-06	7.13E-04	5.84E-14	7.13E-04	2.27E-07	7.15E-04	-3.146	6.02E 03
5.34E-07	5.04E-04	4.13E-14	5.04E-04	8.02E-08	5.05E-04	-3.297	8.51E 03
2.67E-07	3.57E-04	2.92E-14	3.57E-04	2.84E-08	3.57E-04	-3.447	1.20E 04
1.34E-07	2.52E-04	2.07E-14	2.52E-04	1.00E-08	2.52E-04	-3.598	1.70E 04
6.68E-08	1.78E-04	1.46E-14	1.78E-04	3.54E-09	1.78E-04	-3.749	2.40E 04
3.34E-08	1.26E-04	1.03E-14	1.26E-04	1.25E-09	1.26E-04	-3.899	3.40E 04
1.67E-08	8.91E-05	7.30E-15	8.91E-05	4.43E-10	8.92E-05	-4.050	4.81E 04
8.34E-09	6.30E-05	5.16E-15	6.30E-05	1.57E-10	6.30E-05	-4.200	6.80E 04
4.17E-09	4.46E-05	3.65E-15	4.46E-05	5.54E-11	4.46E-05	-4.351	9.62E 04
2.09E-09	3.15E-05	2.58E-15	3.15E-05	1.96E-11	3.15E-05	-4.501	1.36E 05
1.04E-09	2.23E-05	1.83E-15	2.23E-05	6.92E-12	2.23E-05	-4.652	1.92E 05
5.22E-10	1.58E-05	1.29E-15	1.58E-05	2.45E-12	1.58E-05	-4.802	2.72E 05
2.61E-10	1.11E-05	9.13E-16	1.11E-05	8.65E-13	1.11E-05	-4.953	3.85E 05
1.30E-10	7.88E-06	6.45E-16	7.88E-06	3.06E-13	7.88E-06	-5.103	5.44E 05
6.52E-11	5.57E-06	4.56E-16	5.57E-06	1.08E-13	5.57E-06	-5.254	7.69E 05
3.26E-11	3.94E-06	3.23E-16	3.94E-06	3.82E-14	3.94E-06	-5.405	1.09E 06
1.63E-11	2.79E-06	2.28E-16	2.79E-06	1.35E-14	2.79E-06	-5.555	1.54E 06
8.15E-12	1.97E-06	1.61E-16	1.97E-06	4.78E-15	1.97E-06	-5.706	2.18E 06
4.07E-12	1.39E-06	1.14E-16	1.39E-06	1.69E-15	1.39E-06	-5.856	3.08E 06
2.04E-12	9.85E-07	8.07E-17	9.85E-07	5.98E-16	9.85E-07	-6.007	4.35E 06
1.02E-12	6.96E-07	5.70E-17	6.96E-07	2.11E-16	6.96E-07	-6.157	6.15E 06
5.09E-13	4.92E-07	4.03E-17	4.92E-07	7.47E-17	4.92E-07	-6.308	8.70E 06
2.55E-13	3.48E-07	2.85E-17	3.48E-07	2.64E-17	3.48E-07	-6.458	1.23E 07
1.27E-13	2.46E-07	2.02E-17	2.46E-07	9.34E-18	2.46E-07	-6.609	1.74E 07
6.37E-14	1.74E-07	1.43E-17	1.74E-07	3.30E-18	1.74E-07	-6.759	2.46E 07
3.18E-14	1.23E-07	1.01E-17	1.23E-07	1.17E-18	1.23E-07	-6.910	3.48E 07

Table 27. Results of Calculations, t = 125°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 5.0
K1 = 6.69E 00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	4.90E-03	3.78E-09	4.54E-04	4.44E-03	4.51E-02	-1.345	8.44E 00
1.79E-02	2.56E-03	1.98E-09	4.34E-04	2.13E-03	2.26E-02	-1.646	8.44E 00
8.95E-03	1.38E-03	1.07E-09	4.02E-04	9.83E-04	1.13E-02	-1.946	8.46E 00
4.47E-03	7.86E-04	6.07E-10	3.54E-04	4.33E-04	5.69E-03	-2.245	8.51E 00
2.24E-03	4.73E-04	3.66E-10	2.94E-04	1.80E-04	2.89E-03	-2.539	8.64E 00
1.12E-03	3.01E-04	2.33E-10	2.31E-04	7.06E-05	1.49E-03	-2.827	8.91E 00
5.59E-04	2.00E-04	1.55E-10	1.74E-04	2.66E-05	7.86E-04	-3.105	9.40E 00
2.80E-04	1.37E-04	1.06E-10	1.27E-04	9.72E-06	4.26E-04	-3.370	1.02E 01
1.40E-04	9.50E-05	7.34E-11	9.15E-05	3.50E-06	2.38E-04	-3.623	1.14E 01
6.99E-05	6.65E-05	5.14E-11	6.53E-05	1.25E-06	1.38E-04	-3.861	1.32E 01
3.50E-05	4.69E-05	3.62E-11	4.64E-05	4.43E-07	8.22E-05	-4.085	1.57E 01
1.75E-05	3.30E-05	2.55E-11	3.29E-05	1.57E-07	5.07E-05	-4.295	1.94E 01
8.74E-06	2.33E-05	1.80E-11	2.33E-05	5.56E-08	3.21E-05	-4.493	2.46E 01
4.37E-06	1.65E-05	1.27E-11	1.65E-05	1.97E-08	2.09E-05	-4.680	3.20E 01
2.19E-06	1.17E-05	9.00E-12	1.16E-05	6.96E-09	1.38E-05	-4.859	4.24E 01
1.09E-06	8.24E-06	6.37E-12	8.24E-06	2.46E-09	9.33E-06	-5.030	5.72E 01
5.46E-07	5.83E-06	4.50E-12	5.83E-06	8.70E-10	6.37E-06	-5.196	7.81E 01
2.73E-07	4.12E-06	3.18E-12	4.12E-06	3.08E-10	4.39E-06	-5.357	1.08E 02
1.37E-07	2.91E-06	2.25E-12	2.91E-06	1.09E-10	3.05E-06	-5.516	1.49E 02
6.83E-08	2.06E-06	1.59E-12	2.06E-06	3.85E-11	2.13E-06	-5.672	2.08E 02
3.41E-08	1.46E-06	1.13E-12	1.46E-06	1.36E-11	1.49E-06	-5.827	2.92E 02
1.71E-08	1.03E-06	7.96E-13	1.03E-06	4.81E-12	1.05E-06	-5.980	4.10E 02
8.54E-09	7.28E-07	5.63E-13	7.28E-07	1.70E-12	7.37E-07	-6.133	5.77E 02
4.27E-09	5.15E-07	3.98E-13	5.15E-07	6.01E-13	5.19E-07	-6.285	8.14E 02
2.13E-09	3.64E-07	2.81E-13	3.64E-07	2.12E-13	3.66E-07	-6.436	1.15E 03
1.07E-09	2.57E-07	1.99E-13	2.57E-07	7.51E-14	2.59E-07	-6.587	1.62E 03
5.33E-10	1.82E-07	1.41E-13	1.82E-07	2.66E-14	1.83E-07	-6.739	2.29E 03
2.67E-10	1.29E-07	9.95E-14	1.29E-07	9.39E-15	1.29E-07	-6.889	3.24E 03
1.33E-10	9.10E-08	7.03E-14	9.10E-08	3.32E-15	9.12E-08	-7.040	4.57E 03
6.67E-11	6.44E-08	4.97E-14	6.44E-08	1.17E-15	6.44E-08	-7.191	6.46E 03
3.33E-11	4.55E-08	3.52E-14	4.55E-08	4.15E-16	4.55E-08	-7.342	9.14E 03
1.67E-11	3.22E-08	2.49E-14	3.22E-08	1.47E-16	3.22E-08	-7.492	1.29E 04
8.34E-12	2.28E-08	1.76E-14	2.28E-08	5.19E-17	2.28E-08	-7.643	1.83E 04
4.17E-12	1.61E-08	1.24E-14	1.61E-08	1.83E-17	1.61E-08	-7.793	2.58E 04
2.08E-12	1.14E-08	8.79E-15	1.14E-08	6.48E-18	1.14E-08	-7.944	3.65E 04
1.04E-12	8.05E-09	4.22E-15	8.05E-09	2.29E-18	8.05E-09	-8.094	5.17E 04
5.21E-13	5.69E-09	4.40E-15	5.69E-09	8.10E-19	5.69E-09	-8.245	7.31E 04
2.60E-13	4.02E-09	3.11E-15	4.02E-09	2.87E-19	4.02E-09	-8.395	1.03E 05
1.30E-13	2.84E-09	2.20E-15	2.84E-09	1.01E-19	2.84E-09	-8.546	1.46E 05
6.51E-14	2.01E-09	1.55E-15	2.01E-09	3.58E-20	2.01E-09	-8.696	2.07E 05

Table 28. Results of Calculations, t = 125°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 7.0
K1 = 6.69E-00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	4.90E-02	3.78E-10	4.54E-03	4.45E-02	1.29E-01	-0.888	2.42E 01
1.79E-02	2.56E-02	1.98E-10	4.35E-03	2.13E-02	6.48E-02	-1.189	2.42E 01
8.95E-03	1.39E-02	1.07E-10	4.02E-03	9.83E-03	3.26E-02	-1.486	2.44E 01
4.47E-03	7.37E-03	6.07E-11	3.54E-03	4.33E-03	1.67E-02	-1.778	2.49E 01
2.24E-03	4.74E-03	3.66E-11	2.94E-03	1.80E-03	8.77E-03	-2.057	2.62E 01
1.12E-03	3.01E-03	2.33E-11	2.31E-03	7.06E-04	4.84E-03	-2.315	2.89E 01
5.59E-04	2.00E-03	1.55E-11	1.74E-03	2.66E-04	2.83E-03	-2.549	3.38E 01
2.80E-04	1.37E-03	1.06E-11	1.27E-03	9.72E-05	1.75E-03	-2.758	4.17E 01
1.40E-04	9.50E-04	7.33E-12	9.15E-04	3.50E-05	1.12E-03	-2.949	5.38E 01
6.99E-05	6.66E-04	5.14E-12	6.53E-04	1.25E-05	7.48E-04	-3.126	7.16E 01
3.50E-05	4.68E-04	3.62E-12	4.64E-04	4.44E-06	5.08E-04	-3.294	9.72E 01
1.75E-05	3.30E-04	2.55E-12	3.29E-04	1.57E-06	3.50E-04	-3.457	1.34E 02
8.74E-06	2.33E-04	1.80E-12	2.33E-04	5.57E-07	2.43E-04	-3.615	1.86E 02
4.37E-06	1.65E-04	1.27E-12	1.65E-04	1.97E-07	1.70E-04	-3.771	2.59E 02
2.19E-06	1.17E-04	9.00E-13	1.17E-04	6.96E-08	1.19E-04	-3.925	3.64E 02
1.09E-06	8.24E-05	6.36E-13	8.24E-05	2.46E-08	8.36E-05	-4.078	5.12E 02
5.46E-07	5.83E-05	4.50E-13	5.83E-05	8.71E-09	5.88E-05	-4.230	7.21E 02
2.73E-07	4.12E-05	3.18E-13	4.12E-05	3.08E-09	4.15E-05	-4.382	1.02E 03
1.37E-07	2.91E-05	2.25E-13	2.91E-05	1.09E-09	2.93E-05	-4.533	1.43E 03
6.83E-08	2.06E-05	1.59E-13	2.06E-05	3.85E-10	2.07E-05	-4.685	2.03E 03
3.41E-08	1.46E-05	1.12E-13	1.46E-05	1.36E-10	1.46E-05	-4.836	2.86E 03
1.71E-08	1.03E-05	7.95E-14	1.03E-05	4.81E-11	1.03E-05	-4.986	4.04E 03
8.54E-09	7.29E-06	5.62E-14	7.29E-06	1.70E-11	7.29E-06	-5.137	5.72E 03
4.27E-09	5.15E-06	3.98E-14	5.15E-06	6.01E-12	5.16E-06	-5.288	8.08E 03
2.13E-09	3.64E-06	2.81E-14	3.64E-06	2.13E-12	3.64E-06	-5.438	1.14E 04
1.07E-09	2.58E-06	1.99E-14	2.58E-06	7.51E-13	2.58E-06	-5.589	1.62E 04
5.33E-10	1.82E-06	1.41E-14	1.82E-06	2.66E-13	1.82E-06	-5.739	2.28E 04
2.67E-10	1.29E-06	9.94E-15	1.29E-06	9.39E-14	1.29E-06	-5.890	3.23E 04
1.33E-10	9.11E-07	7.03E-15	9.11E-07	3.32E-14	9.11E-07	-6.041	4.57E 04
6.67E-11	6.44E-07	4.97E-15	6.44E-07	1.17E-14	6.44E-07	-6.191	6.46E 04
3.33E-11	4.55E-07	3.51E-15	4.55E-07	4.15E-15	4.55E-07	-6.342	9.14E 04
1.67E-11	3.22E-07	2.49E-15	3.22E-07	1.47E-15	3.22E-07	-6.492	1.29E 05
8.34E-12	2.28E-07	1.76E-15	2.28E-07	5.19E-16	2.28E-07	-6.643	1.83E 05
4.17E-12	1.61E-07	1.24E-15	1.61E-07	1.83E-16	1.61E-07	-6.793	2.58E 05
2.08E-12	1.14E-07	8.79E-16	1.14E-07	6.49E-17	1.14E-07	-6.944	3.65E 05
1.04E-12	8.05E-08	6.21E-16	8.05E-08	2.29E-17	8.05E-08	-7.094	5.17E 05
5.21E-13	5.69E-08	4.39E-16	5.69E-08	8.11E-18	5.69E-08	-7.245	7.31E 05
2.60E-13	4.02E-08	3.11E-16	4.02E-08	2.87E-18	4.02E-08	-7.395	1.03E 06
1.30E-13	2.85E-08	2.20E-16	2.85E-08	1.01E-18	2.85E-08	-7.546	1.46E 06
6.51E-14	2.01E-08	1.55E-16	2.01E-08	3.58E-19	2.01E-08	-7.696	2.07E 06

Table 29. Results of Calculations, t = 125°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 8.0
K1 = 6.69E 00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	1.55E-01	1.20E-10	1.44E-02	1.41E-01	3.31E-01	-0.480	6.19E 01
1.79E-02	8.10E-02	6.25E-11	1.37E-02	6.73E-02	1.66E-01	-0.779	6.21E 01
8.95E-03	4.38E-02	3.38E-11	1.27E-02	3.11E-02	8.39E-02	-1.076	6.27E 01
4.47E-03	2.49E-02	1.92E-11	1.12E-02	1.37E-02	4.30E-02	-1.366	6.44E 01
2.24E-03	1.50E-02	1.16E-11	9.29E-03	5.69E-03	2.29E-02	-1.640	6.85E 01
1.12E-03	9.53E-03	7.36E-12	7.30E-03	2.23E-03	1.29E-02	-1.890	7.71E 01
5.59E-04	6.33E-03	4.89E-12	5.49E-03	8.40E-04	7.73E-03	-2.112	9.25E 01
2.80E-04	4.33E-03	3.34E-12	4.02E-03	3.07E-04	4.91E-03	-2.308	1.18E 02
1.40E-04	3.01E-03	2.32E-12	2.89E-03	1.11E-04	3.26E-03	-2.487	1.56E 02
6.99E-05	2.11E-03	1.62E-12	2.07E-03	3.95E-05	2.21E-03	-2.655	2.12E 02
3.50E-05	1.48E-03	1.14E-12	1.47E-03	1.40E-05	1.53E-03	-2.815	2.93E 02
1.75E-05	1.05E-03	8.07E-13	1.04E-03	4.97E-06	1.07E-03	-2.972	4.09E 02
8.74E-06	7.38E-04	5.70E-13	7.36E-04	1.76E-06	7.49E-04	-3.126	5.73E 02
4.37E-06	5.22E-04	4.03E-13	5.21E-04	6.23E-07	5.27E-04	-3.278	8.06E 02
2.19E-06	3.69E-04	2.85E-13	3.69E-04	2.20E-07	3.71E-04	-3.430	1.14E 03
1.09E-06	2.61E-04	2.01E-13	2.61E-04	7.79E-08	2.62E-04	-3.582	1.60E 03
5.46E-07	1.84E-04	1.42E-13	1.84E-04	2.75E-08	1.85E-04	-3.733	2.26E 03
2.73E-07	1.30E-04	1.01E-13	1.30E-04	9.74E-09	1.31E-04	-3.884	3.20E 03
1.37E-07	9.22E-05	7.11E-14	9.22E-05	3.44E-09	9.23E-05	-4.035	4.52E 03
6.83E-08	6.52E-05	5.03E-14	6.52E-05	1.22E-09	6.52E-05	-4.185	6.39E 03
3.41E-08	4.61E-05	3.56E-14	4.61E-05	4.30E-10	4.61E-05	-4.336	9.04E 03
1.71E-08	3.26E-05	2.51E-14	3.26E-05	1.52E-10	3.26E-05	-4.487	1.28E 04
8.54E-09	2.30E-05	1.78E-14	2.30E-05	5.38E-11	2.31E-05	-4.637	1.81E 04
4.27E-09	1.63E-05	1.26E-14	1.63E-05	1.90E-11	1.63E-05	-4.788	2.55E 04
2.13E-09	1.15E-05	8.89E-15	1.15E-05	6.72E-12	1.15E-05	-4.938	3.61E 04
1.07E-09	8.15E-06	6.29E-15	8.15E-06	2.38E-12	8.15E-06	-5.089	5.11E 04
5.33E-10	5.76E-06	4.45E-15	5.76E-06	8.40E-13	5.76E-06	-5.239	7.22E 04
2.67E-10	4.07E-06	3.14E-15	4.07E-06	2.97E-13	4.07E-06	-5.390	1.02E 05
1.33E-10	2.88E-06	2.22E-15	2.88E-06	1.05E-13	2.88E-06	-5.541	1.44E 05
6.67E-11	2.04E-06	1.57E-15	2.04E-06	3.71E-14	2.04E-06	-5.691	2.04E 05
3.33E-11	1.44E-06	1.11E-15	1.44E-06	1.31E-14	1.44E-06	-5.842	2.89E 05
1.67E-11	1.02E-06	7.86E-16	1.02E-06	4.64E-15	1.02E-06	-5.992	4.09E 05
8.34E-12	7.20E-07	5.56E-16	7.20E-07	1.64E-15	7.20E-07	-6.143	5.78E 05
4.17E-12	5.09E-07	3.93E-16	5.09E-07	5.80E-16	5.09E-07	-6.293	8.17E 05
2.08E-12	3.60E-07	2.78E-16	3.60E-07	2.05E-16	3.60E-07	-6.444	1.16E 06
1.04E-12	2.55E-07	1.96E-16	2.55E-07	7.25E-17	2.55E-07	-6.594	1.63E 06
5.21E-13	1.80E-07	1.39E-16	1.80E-07	2.56E-17	1.80E-07	-6.745	2.31E 06
2.60E-13	1.27E-07	9.82E-17	1.27E-07	9.07E-18	1.27E-07	-6.895	3.27E 06
1.30E-13	9.00E-08	6.95E-17	9.00E-08	3.21E-18	9.00E-08	-7.046	4.62E 06
6.51E-14	6.36E-08	4.91E-17	6.36E-08	1.13E-18	6.36E-08	-7.196	6.54E 06

Table 30. Results of Calculations, t = 125°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 9.0
K1 = 6.69E 00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	4.90E-01	3.78E-11	4.54E-02	4.45E-01	9.71E-01	-0.013	1.81E 02
1.79E-02	2.56E-01	1.98E-11	4.35E-02	2.13E-01	4.87E-01	-0.313	1.82E 02
8.95E-03	1.39E-01	1.07E-11	4.02E-02	9.84E-02	2.46E-01	-0.609	1.84E 02
4.47E-03	7.37E-02	6.07E-12	3.54E-02	4.33E-02	1.26E-01	-0.898	1.89E 02
2.24E-03	4.74E-02	3.65E-12	2.94E-02	1.80E-02	6.76E-02	-1.170	2.02E 02
1.12E-03	3.02E-02	2.33E-12	2.31E-02	7.06E-03	3.83E-02	-1.416	2.29E 02
5.59E-04	2.00E-02	1.55E-12	1.74E-02	2.66E-03	2.33E-02	-1.634	2.78E 02
2.80E-04	1.37E-02	1.06E-12	1.27E-02	9.73E-04	1.49E-02	-1.826	3.57E 02
1.40E-04	9.51E-03	7.33E-13	9.16E-03	3.50E-04	1.00E-02	-2.000	4.78E 02
6.99E-05	6.66E-03	5.14E-13	6.53E-03	1.25E-04	6.85E-03	-2.164	6.56E 02
3.50E-05	4.69E-03	3.61E-13	4.64E-03	4.44E-05	4.77E-03	-2.322	9.12E 02
1.75E-05	3.31E-03	2.55E-13	3.29E-03	1.57E-05	3.34E-03	-2.476	1.28E 03
8.74E-06	2.33E-03	1.80E-13	2.33E-03	5.57E-06	2.35E-03	-2.629	1.80E 03
4.37E-06	1.65E-03	1.27E-13	1.65E-03	1.97E-06	1.66E-03	-2.781	2.54E 03
2.19E-06	1.17E-03	9.00E-14	1.17E-03	6.97E-07	1.17E-03	-2.932	3.58E 03
1.09E-06	8.25E-04	6.36E-14	8.24E-04	2.46E-07	8.26E-04	-3.083	5.06E 03
5.46E-07	5.83E-04	4.50E-14	5.83E-04	8.71E-08	5.84E-04	-3.234	7.15E 03
2.73E-07	4.12E-04	3.18E-14	4.12E-04	3.08E-08	4.13E-04	-3.384	1.01E 04
1.37E-07	2.92E-04	2.25E-14	2.92E-04	1.09E-08	2.92E-04	-3.535	1.43E 04
6.83E-08	2.06E-04	1.59E-14	2.06E-04	3.85E-09	2.06E-04	-3.686	2.02E 04
3.41E-08	1.46E-04	1.12E-14	1.46E-04	1.36E-09	1.46E-04	-3.836	2.86E 04
1.71E-08	1.03E-04	7.95E-15	1.03E-04	4.81E-10	1.03E-04	-3.987	4.04E 04
8.54E-09	7.29E-05	5.62E-15	7.29E-05	1.70E-10	7.29E-05	-4.137	5.71E 04
4.27E-09	5.15E-05	3.97E-15	5.15E-05	6.01E-11	5.15E-05	-4.288	8.08E 04
2.13E-09	3.64E-05	2.81E-15	3.64E-05	2.13E-11	3.64E-05	-4.438	1.14E 05
1.07E-09	2.58E-05	1.99E-15	2.58E-05	7.52E-12	2.58E-05	-4.589	1.62E 05
5.33E-10	1.82E-05	1.41E-15	1.82E-05	2.66E-12	1.82E-05	-4.739	2.29E 05
2.67E-10	1.29E-05	9.94E-16	1.29E-05	9.40E-13	1.29E-05	-4.890	3.23E 05
1.33E-10	9.11E-06	7.03E-16	9.11E-06	3.32E-13	9.11E-06	-5.040	4.57E 05
6.67E-11	6.44E-06	4.97E-16	6.44E-06	1.17E-13	6.44E-06	-5.191	6.46E 05
3.33E-11	4.56E-06	3.51E-16	4.56E-06	4.15E-14	4.56E-06	-5.342	9.14E 05
1.67E-11	3.22E-06	2.48E-16	3.22E-06	1.47E-14	3.22E-06	-5.492	1.29E 06
8.34E-12	2.28E-06	1.76E-16	2.28E-06	5.19E-15	2.28E-06	-5.643	1.83E 06
4.17E-12	1.61E-06	1.24E-16	1.61E-06	1.84E-15	1.61E-06	-5.793	2.59E 06
2.08E-12	1.14E-06	8.78E-17	1.14E-06	6.49E-16	1.14E-06	-5.944	3.66E 06
1.04E-12	8.05E-07	6.21E-17	8.05E-07	2.29E-16	8.05E-07	-6.094	5.17E 06
5.21E-13	5.69E-07	4.39E-17	5.69E-07	8.11E-17	5.69E-07	-6.245	7.31E 06
2.60E-13	4.03E-07	3.11E-17	4.03E-07	2.87E-17	4.03E-07	-6.395	1.03E 07
1.30E-13	2.85E-07	2.20E-17	2.85E-07	1.01E-17	2.85E-07	-6.546	1.46E 07
6.51E-14	2.01E-07	1.55E-17	2.01E-07	3.58E-18	2.01E-07	-6.696	2.07E 07

Table 31. Results of Calculations, t = 125°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 9.2
K1 = 6.60E 00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	6.17E-01	3.00E-11	5.72E-02	5.60E-01	1.21E 00	0.084	2.27E 02
1.79E-02	3.23E-01	1.57E-11	5.47E-02	2.68E-01	6.08E-01	-0.216	2.27E 02
8.95E-03	1.74E-01	8.49E-12	5.06E-02	1.24E-01	3.07E-01	-0.513	2.30E 02
4.47E-03	9.91E-02	4.82E-12	4.46E-02	5.45E-02	1.58E-01	-0.801	2.36E 02
2.24E-03	5.96E-02	2.90E-12	3.70E-02	2.26E-02	8.45E-02	-1.073	2.53E 02
1.12E-03	3.80E-02	1.85E-12	2.91E-02	8.89E-03	4.80E-02	-1.319	2.87E 02
5.59E-04	2.52E-02	1.23E-12	2.19E-02	3.35E-03	2.91E-02	-1.536	3.48E 02
2.80E-04	1.72E-02	8.39E-13	1.60E-02	1.22E-03	1.87E-02	-1.727	4.48E 02
1.40E-04	1.20E-02	5.82E-13	1.15E-02	4.41E-04	1.25E-02	-1.901	6.00E 02
6.99E-05	8.38E-03	4.08E-13	8.23E-03	1.57E-04	8.61E-03	-2.065	8.24E 02
3.50E-05	5.90E-03	2.87E-13	5.84E-03	5.59E-05	5.99E-03	-2.222	1.15E 03
1.75E-05	4.16E-03	2.03E-13	4.14E-03	1.98E-05	4.20E-03	-2.377	1.61E 03
8.74E-06	2.94E-03	1.43E-13	2.93E-03	7.01E-06	2.96E-03	-2.529	2.26E 03
4.37E-06	2.08E-03	1.01E-13	2.07E-03	2.48E-06	2.08E-03	-2.681	3.19E 03
2.19E-06	1.47E-03	7.15E-14	1.47E-03	8.77E-07	1.47E-03	-2.832	4.51E 03
1.09E-06	1.04E-03	5.05E-14	1.04E-03	3.10E-07	1.04E-03	-2.983	6.37E 03
5.46E-07	7.34E-04	3.57E-14	7.34E-04	1.10E-07	7.35E-04	-3.134	9.00E 03
2.73E-07	5.19E-04	2.53E-14	5.19E-04	3.88E-08	5.19E-04	-3.285	1.27E 04
1.37E-07	3.67E-04	1.79E-14	3.67E-04	1.37E-08	3.67E-04	-3.435	1.80E 04
6.83E-08	2.60E-04	1.26E-14	2.60E-04	4.85E-09	2.60E-04	-3.586	2.54E 04
3.41E-08	1.84E-04	8.93E-15	1.84E-04	1.71E-09	1.84E-04	-3.736	3.60E 04
1.71E-08	1.30E-04	6.31E-15	1.30E-04	6.06E-10	1.30E-04	-3.887	5.09E 04
8.54E-09	9.13E-05	4.47E-15	9.18E-05	2.14E-10	9.18E-05	-4.037	7.19E 04
4.27E-09	6.49E-05	3.16E-15	6.49E-05	7.57E-11	6.49E-05	-4.188	1.02E 05
2.13E-09	4.59E-05	2.23E-15	4.59E-05	2.68E-11	4.59E-05	-4.338	1.44E 05
1.07E-09	3.24E-05	1.58E-15	3.24E-05	9.46E-12	3.24E-05	-4.489	2.03E 05
5.33E-10	2.29E-05	1.12E-15	2.29E-05	3.35E-12	2.29E-05	-4.639	2.88E 05
2.67E-10	1.62E-05	7.89E-16	1.62E-05	1.18E-12	1.62E-05	-4.790	4.07E 05
1.33E-10	1.15E-05	5.58E-16	1.15E-05	4.18E-13	1.15E-05	-4.940	5.75E 05
6.67E-11	8.11E-06	3.95E-16	8.11E-06	1.48E-13	8.11E-06	-5.091	8.14E 05
3.33E-11	5.73E-06	2.79E-16	5.73E-06	5.23E-14	5.73E-06	-5.241	1.15E 06
1.67E-11	4.06E-06	1.97E-16	4.06E-06	1.85E-14	4.06E-06	-5.392	1.63E 06
8.34E-12	2.87E-06	1.40E-16	2.87E-06	6.54E-15	2.87E-06	-5.543	2.30E 06
4.17E-12	2.03E-06	9.87E-17	2.03E-06	2.31E-15	2.03E-06	-5.693	3.25E 06
2.08E-12	1.43E-06	6.98E-17	1.43E-06	8.17E-16	1.43E-06	-5.844	4.60E 06
1.04E-12	1.01E-06	4.93E-17	1.01E-06	2.89E-16	1.01E-06	-5.994	6.51E 06
5.21E-13	7.17E-07	3.49E-17	7.17E-07	1.02E-16	7.17E-07	-6.145	9.21E 06
2.60E-13	5.07E-07	2.47E-17	5.07E-07	3.61E-17	5.07E-07	-6.295	1.30E 07
1.30E-13	3.58E-07	1.74E-17	3.58E-07	1.28E-17	3.58E-07	-6.446	1.84E 07
6.51E-14	2.53E-07	1.23E-17	2.53E-07	4.51E-18	2.53E-07	-6.596	2.60E 07

Table 32. Results of Calculations, t = 125°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 125.0 DEG C PH = 9.5
K1 = 6.69E 00 K2 = 2.73E 02 K3 = 6.20E-10 K4 = 4.80E-11
SOLUBILITY OF I2 IN WATER = 3.58E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
3.58E-02	8.72E-01	2.13E-11	3.08E-02	7.91E-01	1.70E 00	0.230	3.17E 02
1.79E-02	4.55E-01	1.11E-11	7.73E-02	3.78E-01	8.52E-01	-0.070	3.18E 02
8.95E-03	2.46E-01	6.01E-12	7.15E-02	1.75E-01	4.30E-01	-0.366	3.22E 02
4.47E-03	1.40E-01	3.41E-12	6.29E-02	7.70E-02	2.21E-01	-0.655	3.31E 02
2.24E-03	8.43E-02	2.05E-12	5.23E-02	3.20E-02	1.18E-01	-0.926	3.54E 02
1.12E-03	5.36E-02	1.31E-12	4.11E-02	1.26E-02	6.73E-02	-1.172	4.02E 02
5.59E-04	3.56E-02	8.69E-13	3.09E-02	4.73E-03	4.09E-02	-1.388	4.89E 02
2.80E-04	2.43E-02	5.94E-13	2.26E-02	1.73E-03	2.64E-02	-1.579	6.30E 02
1.40E-04	1.69E-02	4.12E-13	1.63E-02	6.23E-04	1.77E-02	-1.753	8.45E 02
6.99E-05	1.18E-02	2.89E-13	1.16E-02	2.22E-04	1.21E-02	-1.916	1.16E 03
3.50E-05	8.34E-03	2.03E-13	8.26E-03	7.89E-05	8.45E-03	-2.073	1.62E 03
1.75E-05	5.88E-03	1.43E-13	5.85E-03	2.80E-05	5.93E-03	-2.227	2.27E 03
8.74E-06	4.15E-03	1.01E-13	4.14E-03	9.90E-06	4.17E-03	-2.380	3.19E 03
4.37E-06	2.93E-03	7.16E-14	2.93E-03	3.50E-06	2.94E-03	-2.531	4.50E 03
2.19E-06	2.07E-03	5.06E-14	2.07E-03	1.24E-06	2.08E-03	-2.682	6.36E 03
1.09E-06	1.47E-03	3.58E-14	1.47E-03	4.38E-07	1.47E-03	-2.833	8.99E 03
5.46E-07	1.04E-03	2.53E-14	1.04E-03	1.55E-07	1.04E-03	-2.984	1.27E 04
2.73E-07	7.33E-04	1.79E-14	7.33E-04	5.48E-08	7.34E-04	-3.135	1.80E 04
1.37E-07	5.18E-04	1.26E-14	5.18E-04	1.94E-08	5.19E-04	-3.285	2.54E 04
6.83E-08	3.67E-04	8.94E-15	3.67E-04	6.85E-09	3.67E-04	-3.436	3.59E 04
3.41E-08	2.59E-04	6.32E-15	2.59E-04	2.42E-09	2.59E-04	-3.586	5.08E 04
1.71E-08	1.83E-04	4.47E-15	1.83E-04	8.56E-10	1.83E-04	-3.737	7.18E 04
8.54E-09	1.30E-04	3.16E-15	1.30E-04	3.03E-10	1.30E-04	-3.887	1.02E 05
4.27E-09	9.17E-05	2.24E-15	9.17E-05	1.07E-10	9.17E-05	-4.038	1.44E 05
2.13E-09	6.48E-05	1.58E-15	6.48E-05	3.78E-11	6.48E-05	-4.188	2.03E 05
1.07E-09	4.58E-05	1.12E-15	4.58E-05	1.34E-11	4.58E-05	-4.339	2.87E 05
5.33E-10	3.24E-05	7.90E-16	3.24E-05	4.73E-12	3.24E-05	-4.489	4.06E 05
2.67E-10	2.29E-05	5.59E-16	2.29E-05	1.67E-12	2.29E-05	-4.640	5.75E 05
1.33E-10	1.62E-05	3.95E-16	1.62E-05	5.91E-13	1.62E-05	-4.790	8.13E 05
6.67E-11	1.15E-05	2.79E-16	1.15E-05	2.09E-13	1.15E-05	-4.941	1.15E 06
3.33E-11	8.10E-06	1.98E-16	8.10E-06	7.39E-14	8.10E-06	-5.091	1.63E 06
1.67E-11	5.73E-06	1.40E-16	5.73E-06	2.61E-14	5.73E-06	-5.242	2.30E 06
8.34E-12	4.05E-06	9.88E-17	4.05E-06	9.23E-15	4.05E-06	-5.392	3.25E 06
4.17E-12	2.86E-06	6.98E-17	2.86E-06	3.26E-15	2.86E-06	-5.543	4.60E 06
2.08E-12	2.03E-06	4.94E-17	2.03E-06	1.15E-15	2.03E-06	-5.694	6.50E 06
1.04E-12	1.43E-06	3.49E-17	1.43E-06	4.08E-16	1.43E-06	-5.844	9.20E 06
5.21E-13	1.01E-06	2.47E-17	1.01E-06	1.44E-16	1.01E-06	-5.995	1.30E 07
2.60E-13	7.16E-07	1.75E-17	7.16E-07	5.10E-17	7.16E-07	-6.145	1.84E 07
1.30E-13	5.06E-07	1.23E-17	5.06E-07	1.80E-17	5.06E-07	-6.296	2.60E 07
6.51E-14	3.58E-07	8.73E-18	3.58E-07	6.38E-18	3.58E-07	-6.446	3.68E 07

Table 33. Results of Calculations, t = 150°C, pH = 5.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 5.0
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	1.49E-02	4.24E-09	8.37E-04	1.41E-02	9.11E-02	-1.040	8.09E 00
3.11E-02	7.65E-03	2.18E-09	8.15E-04	6.84E-03	4.56E-02	-1.341	8.09E 00
1.55E-02	4.02E-03	1.14E-09	7.74E-04	3.25E-03	2.28E-02	-1.642	8.10E 00
7.77E-03	2.20E-03	6.25E-10	7.09E-04	1.49E-03	1.15E-02	-1.941	8.14E 00
3.89E-03	1.26E-03	3.59E-10	6.17E-04	6.47E-04	5.80E-03	-2.237	8.23E 00
1.94E-03	7.71E-04	2.19E-10	5.05E-04	2.65E-04	2.98E-03	-2.526	8.46E 00
9.72E-04	4.96E-04	1.41E-10	3.93E-04	1.03E-04	1.57E-03	-2.804	8.92E 00
4.86E-04	3.32E-04	9.44E-11	2.93E-04	3.85E-05	8.56E-04	-3.067	9.73E 00
2.43E-04	2.28E-04	6.48E-11	2.14E-04	1.40E-05	4.85E-04	-3.314	1.10E 01
1.21E-04	1.59E-04	4.51E-11	1.54E-04	5.03E-06	2.85E-04	-3.545	1.30E 01
6.07E-05	1.11E-04	3.16E-11	1.09E-04	1.79E-06	1.74E-04	-3.760	1.58E 01
3.04E-05	7.33E-05	2.23E-11	7.77E-05	6.37E-07	1.09E-04	-3.961	1.99E 01
1.52E-05	5.53E-05	1.57E-11	5.51E-05	2.26E-07	7.07E-05	-4.151	2.57E 01
7.59E-06	3.90E-05	1.11E-11	3.90E-05	7.99E-08	4.67E-05	-4.330	3.40E 01
3.80E-06	2.76E-05	7.85E-12	2.76E-05	2.82E-08	3.14E-05	-4.503	4.57E 01
1.90E-06	1.95E-05	5.55E-12	1.95E-05	9.99E-09	2.14E-05	-4.669	6.23E 01
9.49E-07	1.38E-05	3.92E-12	1.38E-05	3.53E-09	1.47E-05	-4.831	8.58E 01
4.75E-07	9.75E-06	2.77E-12	9.75E-06	1.25E-09	1.02E-05	-4.990	1.19E 02
2.37E-07	6.90E-06	1.96E-12	6.90E-06	4.42E-10	7.13E-06	-5.147	1.66E 02
1.19E-07	4.88E-06	1.39E-12	4.88E-06	1.56E-10	4.99E-06	-5.301	2.32E 02
5.93E-08	3.45E-06	9.81E-13	3.45E-06	5.52E-11	3.51E-06	-5.455	3.26E 02
2.97E-08	2.44E-06	6.93E-13	2.44E-06	1.95E-11	2.47E-06	-5.608	4.59E 02
1.48E-08	1.72E-06	4.90E-13	1.72E-06	6.90E-12	1.74E-06	-5.760	6.47E 02
7.41E-09	1.22E-06	3.47E-13	1.22E-06	2.44E-12	1.23E-06	-5.911	9.13E 02
3.71E-09	8.62E-07	2.45E-13	8.62E-07	8.63E-13	8.66E-07	-6.063	1.29E 03
1.85E-09	6.10E-07	1.73E-13	6.10E-07	3.05E-13	6.11E-07	-6.214	1.82E 03
9.27E-10	4.31E-07	1.23E-13	4.31E-07	1.08E-13	4.32E-07	-6.365	2.57E 03
4.63E-10	3.05E-07	8.67E-14	3.05E-07	3.81E-14	3.05E-07	-6.515	3.64E 03
2.32E-10	2.15E-07	6.13E-14	2.15E-07	1.35E-14	2.16E-07	-6.666	5.14E 03
1.16E-10	1.52E-07	4.33E-14	1.52E-07	4.76E-15	1.52E-07	-6.817	7.27E 03
5.79E-11	1.08E-07	3.06E-14	1.08E-07	1.68E-15	1.08E-07	-6.967	1.03E 04
2.90E-11	7.62E-08	2.17E-14	7.62E-08	5.96E-16	7.62E-08	-7.118	1.45E 04
1.45E-11	5.39E-08	1.53E-14	5.39E-08	2.11E-16	5.39E-08	-7.269	2.05E 04
7.24E-12	3.81E-08	1.08E-14	3.81E-08	7.44E-17	3.81E-08	-7.419	2.90E 04
3.62E-12	2.69E-08	7.66E-15	2.69E-08	2.63E-17	2.69E-08	-7.570	4.11E 04
1.81E-12	1.90E-08	5.42E-15	1.90E-08	9.31E-18	1.90E-08	-7.720	5.81E 04
9.05E-13	1.35E-08	3.83E-15	1.35E-08	3.29E-18	1.35E-08	-7.871	8.21E 04
4.53E-13	9.52E-09	2.71E-15	9.52E-09	1.16E-18	9.52E-09	-8.021	1.16E 05
2.26E-13	6.73E-09	1.92E-15	6.73E-09	4.11E-19	6.73E-09	-8.172	1.64E 05
1.13E-13	4.76E-09	1.35E-15	4.76E-09	1.45E-19	4.76E-09	-8.322	2.32E 05

Table 34. Results of Calculations, t = 150°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 7.0
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	1.49E-01	4.23E-10	8.37E-03	1.41E-01	3.52E-01	-0.454	3.12E 01
3.11E-02	7.65E-02	2.18E-10	8.15E-03	6.84E-02	1.76E-01	-0.754	3.12E 01
1.55E-02	4.03E-02	1.14E-10	7.75E-03	3.25E-02	8.83E-02	-1.054	3.14E 01
7.77E-03	2.20E-02	6.25E-11	7.09E-03	1.49E-02	4.46E-02	-1.350	3.17E 01
3.89E-03	1.26E-02	3.59E-11	6.17E-03	6.47E-03	2.30E-02	-1.638	3.27E 01
1.94E-03	7.71E-03	2.19E-11	5.06E-03	2.65E-03	1.23E-02	-1.910	3.49E 01
9.72E-04	4.96E-03	1.41E-11	3.93E-03	1.03E-03	6.96E-03	-2.157	3.95E 01
4.86E-04	3.32E-03	9.44E-12	2.94E-03	3.85E-04	4.19E-03	-2.378	4.76E 01
2.43E-04	2.28E-03	6.48E-12	2.14E-03	1.40E-04	2.66E-03	-2.575	6.05E 01
1.21E-04	1.59E-03	4.51E-12	1.54E-03	5.04E-05	1.76E-03	-2.755	7.99E 01
6.07E-05	1.11E-03	3.16E-12	1.09E-03	1.79E-05	1.19E-03	-2.924	1.08E 02
3.04E-05	7.84E-04	2.23E-12	7.77E-04	6.37E-06	8.20E-04	-3.086	1.49E 02
1.52E-05	5.53E-04	1.57E-12	5.51E-04	2.26E-06	5.70E-04	-3.244	2.07E 02
7.59E-06	3.91E-04	1.11E-12	3.90E-04	7.99E-07	3.99E-04	-3.399	2.90E 02
3.80E-06	2.76E-04	7.85E-13	2.76E-04	2.83E-07	2.80E-04	-3.553	4.07E 02
1.90E-06	1.95E-04	5.55E-13	1.95E-04	9.99E-08	1.97E-04	-3.705	5.73E 02
9.49E-07	1.38E-04	3.92E-13	1.38E-04	3.53E-08	1.39E-04	-3.857	8.08E 02
4.75E-07	9.76E-05	2.77E-13	9.76E-05	1.25E-08	9.81E-05	-4.009	1.14E 03
2.37E-07	6.90E-05	1.96E-13	6.90E-05	4.42E-09	6.92E-05	-4.160	1.61E 03
1.19E-07	4.88E-05	1.39E-13	4.88E-05	1.56E-09	4.89E-05	-4.311	2.28E 03
5.93E-08	3.45E-05	9.80E-14	3.45E-05	5.52E-10	3.46E-05	-4.462	3.22E 03
2.97E-08	2.44E-05	6.93E-14	2.44E-05	1.95E-10	2.44E-05	-4.612	4.55E 03
1.48E-08	1.72E-05	4.90E-14	1.72E-05	6.90E-11	1.73E-05	-4.763	6.43E 03
7.41E-09	1.22E-05	3.47E-14	1.22E-05	2.44E-11	1.22E-05	-4.914	9.08E 03
3.71E-09	8.62E-06	2.45E-14	8.62E-06	8.63E-12	8.63E-06	-5.064	1.28E 04
1.85E-09	6.10E-06	1.73E-14	6.10E-06	3.05E-12	6.10E-06	-5.215	1.82E 04
9.27E-10	4.31E-06	1.23E-14	4.31E-06	1.08E-12	4.31E-06	-5.365	2.57E 04
4.63E-10	3.05E-06	8.66E-15	3.05E-06	3.81E-13	3.05E-06	-5.516	3.63E 04
2.32E-10	2.16E-06	6.13E-15	2.16E-06	1.35E-13	2.16E-06	-5.666	5.14E 04
1.16E-10	1.52E-06	4.33E-15	1.52E-06	4.77E-14	1.52E-06	-5.817	7.26E 04
5.79E-11	1.08E-06	3.06E-15	1.08E-06	1.69E-14	1.08E-06	-5.967	1.03E 05
2.90E-11	7.62E-07	2.17E-15	7.62E-07	5.96E-15	7.62E-07	-6.118	1.45E 05
1.45E-11	5.39E-07	1.53E-15	5.39E-07	2.11E-15	5.39E-07	-6.268	2.05E 05
7.24E-12	3.81E-07	1.08E-15	3.81E-07	7.45E-16	3.81E-07	-6.419	2.91E 05
3.62E-12	2.69E-07	7.66E-16	2.69E-07	2.63E-16	2.69E-07	-6.569	4.11E 05
1.81E-12	1.91E-07	5.42E-16	1.91E-07	9.31E-17	1.91E-07	-6.720	5.81E 05
9.05E-13	1.35E-07	3.83E-16	1.35E-07	3.29E-17	1.35E-07	-6.871	8.22E 05
4.53E-13	9.53E-08	2.71E-16	9.53E-08	1.16E-17	9.53E-08	-7.021	1.16E 06
2.26E-13	6.74E-08	1.91E-16	6.74E-08	4.11E-18	6.74E-08	-7.172	1.64E 06
1.13E-13	4.76E-08	1.35E-16	4.76E-08	1.45E-18	4.76E-08	-7.322	2.32E 06

Table 35. Results of Calculations, t = 150°C, pH = 8.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 8.0
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	4.71E-01	1.34E-10	2.65E-02	4.45E-01	9.78E-01	-0.010	8.68E 01
3.11E-02	2.42E-01	6.88E-11	2.58E-02	2.16E-01	4.90E-01	-0.310	8.69E 01
1.55E-02	1.27E-01	3.62E-11	2.45E-02	1.03E-01	2.46E-01	-0.610	8.72E 01
7.77E-03	6.85E-02	1.97E-11	2.24E-02	4.71E-02	1.24E-01	-0.905	8.83E 01
3.89E-03	4.00E-02	1.14E-11	1.95E-02	2.05E-02	6.43E-02	-1.192	9.14E 01
1.94E-03	2.44E-02	6.93E-12	1.60E-02	8.39E-03	3.47E-02	-1.459	9.86E 01
9.72E-04	1.57E-02	4.46E-12	1.24E-02	3.26E-03	1.99E-02	-1.701	1.13E 02
4.86E-04	1.05E-02	2.98E-12	9.28E-03	1.22E-03	1.22E-02	-1.913	1.39E 02
2.43E-04	7.21E-03	2.05E-12	6.76E-03	4.44E-04	7.89E-03	-2.103	1.79E 02
1.21E-04	5.02E-03	1.43E-12	4.86E-03	1.59E-04	5.30E-03	-2.276	2.41E 02
6.07E-05	3.52E-03	1.00E-12	3.46E-03	5.68E-05	3.64E-03	-2.439	3.31E 02
3.04E-05	2.48E-03	7.04E-13	2.46E-03	2.02E-05	2.53E-03	-2.597	4.60E 02
1.52E-05	1.75E-03	4.97E-13	1.74E-03	7.14E-06	1.77E-03	-2.752	6.44E 02
7.59E-06	1.24E-03	3.51E-13	1.23E-03	2.53E-06	1.25E-03	-2.905	9.06E 02
3.80E-06	8.73E-04	2.48E-13	8.72E-04	8.94E-07	8.78E-04	-3.057	1.28E 03
1.90E-06	6.17E-04	1.75E-13	6.17E-04	3.16E-07	6.20E-04	-3.208	1.80E 03
9.49E-07	4.36E-04	1.24E-13	4.36E-04	1.12E-07	4.38E-04	-3.359	2.54E 03
4.75E-07	3.09E-04	8.77E-14	3.09E-04	3.95E-08	3.09E-04	-3.510	3.60E 03
2.37E-07	2.18E-04	6.20E-14	2.18E-04	1.40E-08	2.18E-04	-3.661	5.08E 03
1.19E-07	1.54E-04	4.38E-14	1.54E-04	4.94E-09	1.54E-04	-3.811	7.18E 03
5.93E-08	1.09E-04	3.10E-14	1.09E-04	1.75E-09	1.09E-04	-3.962	1.02E 04
2.97E-08	7.71E-05	2.19E-14	7.71E-05	6.18E-10	7.72E-05	-4.113	1.44E 04
1.48E-08	5.46E-05	1.55E-14	5.46E-05	2.19E-10	5.46E-05	-4.263	2.03E 04
7.41E-09	3.86E-05	1.10E-14	3.86E-05	7.72E-11	3.86E-05	-4.414	2.87E 04
3.71E-09	2.73E-05	7.75E-15	2.73E-05	2.73E-11	2.73E-05	-4.564	4.06E 04
1.85E-09	1.93E-05	5.48E-15	1.93E-05	9.65E-12	1.93E-05	-4.715	5.74E 04
9.27E-10	1.36E-05	3.87E-15	1.36E-05	3.41E-12	1.36E-05	-4.865	8.12E 04
4.63E-10	9.64E-06	2.74E-15	9.64E-06	1.21E-12	9.64E-06	-5.016	1.15E 05
2.32E-10	6.82E-06	1.94E-15	6.82E-06	4.26E-13	6.82E-06	-5.166	1.62E 05
1.16E-10	4.82E-06	1.37E-15	4.82E-06	1.51E-13	4.82E-06	-5.317	2.30E 05
5.79E-11	3.41E-06	9.68E-16	3.41E-06	5.33E-14	3.41E-06	-5.467	3.25E 05
2.90E-11	2.41E-06	6.85E-16	2.41E-06	1.88E-14	2.41E-06	-5.618	4.59E 05
1.45E-11	1.70E-06	4.84E-16	1.70E-06	6.66E-15	1.70E-06	-5.768	6.50E 05
7.24E-12	1.21E-06	3.42E-16	1.21E-06	2.36E-15	1.21E-06	-5.919	9.19E 05
3.62E-12	8.52E-07	2.42E-16	8.52E-07	8.33E-16	8.52E-07	-6.069	1.30E 06
1.81E-12	6.03E-07	1.71E-16	6.03E-07	2.94E-16	6.03E-07	-6.220	1.84E 06
9.05E-13	4.26E-07	1.21E-16	4.26E-07	1.04E-16	4.26E-07	-6.370	2.60E 06
4.53E-13	3.01E-07	8.56E-17	3.01E-07	3.68E-17	3.01E-07	-6.521	3.68E 06
2.26E-13	2.13E-07	6.05E-17	2.13E-07	1.30E-17	2.13E-07	-6.671	5.20E 06
1.13E-13	1.51E-07	4.28E-17	1.51E-07	4.60E-18	1.51E-07	-6.822	7.35E 06

Table 36. Results of Calculations, t = 150°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 9.0
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	1.49E 00	4.23E-11	8.38E-02	1.41E 00	2.96E 00	0.471	2.63E 02
3.11E-02	7.64E-01	2.17E-11	8.15E-02	6.84E-01	1.48E 00	0.171	2.63E 02
1.55E-02	4.03E-01	1.14E-11	7.75E-02	3.25E-01	7.44E-01	-0.129	2.64E 02
7.77E-03	2.20E-01	6.24E-12	7.10E-02	1.49E-01	3.77E-01	-0.424	2.67E 02
3.89E-03	1.26E-01	3.59E-12	6.17E-02	6.47E-02	1.95E-01	-0.710	2.77E 02
1.94E-03	7.71E-02	2.19E-12	5.06E-02	2.65E-02	1.06E-01	-0.976	3.00E 02
9.72E-04	4.96E-02	1.41E-12	3.93E-02	1.03E-02	6.09E-02	-1.215	3.46E 02
4.86E-04	3.32E-02	9.43E-13	2.94E-02	3.85E-03	3.76E-02	-1.425	4.27E 02
2.43E-04	2.23E-02	6.47E-13	2.14E-02	1.40E-03	2.44E-02	-1.612	5.55E 02
1.21E-04	1.59E-02	4.51E-13	1.54E-02	5.04E-04	1.65E-02	-1.783	7.50E 02
6.07E-05	1.11E-02	3.16E-13	1.10E-02	1.80E-04	1.14E-02	-1.944	1.03E 03
3.04E-05	7.64E-03	2.23E-13	7.78E-03	6.37E-05	7.93E-03	-2.100	1.44E 03
1.52E-05	5.53E-03	1.57E-13	5.51E-03	2.26E-05	5.57E-03	-2.254	2.02E 03
7.59E-06	3.91E-03	1.11E-13	3.90E-03	7.97E-06	3.92E-03	-2.406	2.85E 03
3.80E-06	2.76E-03	7.84E-14	2.76E-03	2.83E-06	2.77E-03	-2.558	4.03E 03
1.90E-06	1.95E-03	5.54E-14	1.95E-03	1.00E-06	1.96E-03	-2.709	5.69E 03
9.49E-07	1.38E-03	3.92E-14	1.38E-03	3.54E-07	1.38E-03	-2.860	8.04E 03
4.75E-07	9.76E-04	2.77E-14	9.76E-04	1.25E-07	9.77E-04	-3.010	1.14E 04
2.37E-07	6.90E-04	1.96E-14	6.90E-04	4.42E-08	6.90E-04	-3.161	1.61E 04
1.19E-07	4.88E-04	1.39E-14	4.88E-04	1.56E-08	4.88E-04	-3.311	2.27E 04
5.93E-08	3.45E-04	9.80E-15	3.45E-04	5.52E-09	3.45E-04	-3.462	3.21E 04
2.97E-08	2.44E-04	6.93E-15	2.44E-04	1.95E-09	2.44E-04	-3.613	4.54E 04
1.48E-08	1.73E-04	4.90E-15	1.73E-04	6.91E-10	1.73E-04	-3.763	6.42E 04
7.41E-09	1.22E-04	3.46E-15	1.22E-04	2.44E-10	1.22E-04	-3.914	9.08E 04
3.71E-09	8.63E-05	2.45E-15	8.63E-05	8.63E-11	8.63E-05	-4.064	1.28E 05
1.85E-09	6.10E-05	1.73E-15	6.10E-05	3.05E-11	6.10E-05	-4.215	1.82E 05
9.27E-10	4.31E-05	1.22E-15	4.31E-05	1.08E-11	4.31E-05	-4.365	2.57E 05
4.63E-10	3.05E-05	8.66E-16	3.05E-05	3.81E-12	3.05E-05	-4.516	3.63E 05
2.32E-10	2.16E-05	6.12E-16	2.16E-05	1.35E-12	2.16E-05	-4.666	5.14E 05
1.16E-10	1.53E-05	4.33E-16	1.53E-05	4.77E-13	1.53E-05	-4.817	7.27E 05
5.79E-11	1.08E-05	3.06E-16	1.08E-05	1.69E-13	1.08E-05	-4.967	1.03E 06
2.90E-11	7.63E-06	2.17E-16	7.63E-06	5.96E-14	7.63E-06	-5.118	1.45E 06
1.45E-11	5.39E-06	1.53E-16	5.39E-06	2.11E-14	5.39E-06	-5.268	2.06E 06
7.24E-12	3.81E-06	1.08E-16	3.81E-06	7.45E-15	3.81E-06	-5.419	2.91E 06
3.62E-12	2.70E-06	7.65E-17	2.70E-06	2.63E-15	2.70E-06	-5.569	4.11E 06
1.81E-12	1.91E-06	5.41E-17	1.91E-06	9.31E-16	1.91E-06	-5.720	5.81E 06
9.05E-13	1.35E-06	3.83E-17	1.35E-06	3.29E-16	1.35E-06	-5.870	8.22E 06
4.53E-13	9.53E-07	2.71E-17	9.53E-07	1.16E-16	9.53E-07	-6.021	1.16E 07
2.26E-13	6.74E-07	1.91E-17	6.74E-07	4.12E-17	6.74E-07	-6.171	1.64E 07
1.13E-13	4.77E-07	1.35E-17	4.77E-07	1.46E-17	4.77E-07	-6.322	2.33E 07

Table 37. Results of Calculations, t = 150°C, pH = 9.2

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 9.2
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	1.88E 00	3.36E-11	1.05E-01	1.77E 00	3.71E 00	0.569	3.29E 02
3.11E-02	9.64E-01	1.73E-11	1.03E-01	8.62E-01	1.86E 00	0.269	3.30E 02
1.55E-02	5.07E-01	9.08E-12	9.76E-02	4.10E-01	9.32E-01	-0.031	3.31E 02
7.77E-03	2.77E-01	4.96E-12	8.94E-02	1.88E-01	4.72E-01	-0.326	3.35E 02
3.89E-03	1.59E-01	2.85E-12	7.77E-02	8.15E-02	2.45E-01	-0.612	3.47E 02
1.94E-03	9.71E-02	1.74E-12	6.37E-02	3.34E-02	1.32E-01	-0.878	3.76E 02
9.72E-04	6.25E-02	1.12E-12	4.95E-02	1.30E-02	7.64E-02	-1.117	4.34E 02
4.86E-04	4.18E-02	7.49E-13	3.70E-02	4.85E-03	4.72E-02	-1.326	5.36E 02
2.43E-04	2.87E-02	5.14E-13	2.69E-02	1.77E-03	3.07E-02	-1.513	6.98E 02
1.21E-04	2.00E-02	3.58E-13	1.93E-02	6.34E-04	2.07E-02	-1.683	9.42E 02
6.07E-05	1.40E-02	2.51E-13	1.38E-02	2.26E-04	1.43E-02	-1.845	1.30E 03
3.04E-05	9.87E-03	1.77E-13	9.79E-03	8.03E-05	9.98E-03	-2.001	1.81E 03
1.52E-05	6.97E-03	1.25E-13	6.94E-03	2.84E-05	7.01E-03	-2.154	2.55E 03
7.59E-06	4.92E-03	8.81E-14	4.91E-03	1.01E-05	4.94E-03	-2.306	3.59E 03
3.80E-06	3.48E-03	6.23E-14	3.47E-03	3.56E-06	3.48E-03	-2.458	5.07E 03
1.90E-06	2.46E-03	4.40E-14	2.46E-03	1.26E-06	2.46E-03	-2.609	7.16E 03
9.49E-07	1.74E-03	3.11E-14	1.74E-03	4.45E-07	1.74E-03	-2.760	1.01E 04
4.75E-07	1.23E-03	2.20E-14	1.23E-03	1.57E-07	1.23E-03	-2.910	1.43E 04
2.37E-07	8.69E-04	1.56E-14	8.69E-04	5.56E-08	8.69E-04	-3.061	2.02E 04
1.19E-07	6.14E-04	1.10E-14	6.14E-04	1.97E-08	6.15E-04	-3.211	2.86E 04
5.93E-08	4.34E-04	7.78E-15	4.34E-04	6.96E-09	4.35E-04	-3.362	4.04E 04
2.97E-08	3.07E-04	5.50E-15	3.07E-04	2.46E-09	3.07E-04	-3.513	5.72E 04
1.48E-08	2.17E-04	3.89E-15	2.17E-04	8.69E-10	2.17E-04	-3.663	8.09E 04
7.41E-09	1.54E-04	2.75E-15	1.54E-04	3.07E-10	1.54E-04	-3.814	1.14E 05
3.71E-09	1.09E-04	1.95E-15	1.09E-04	1.09E-10	1.09E-04	-3.964	1.62E 05
1.85E-09	7.68E-05	1.38E-15	7.68E-05	3.84E-11	7.68E-05	-4.115	2.29E 05
9.27E-10	5.43E-05	9.73E-16	5.43E-05	1.36E-11	5.43E-05	-4.265	3.23E 05
4.63E-10	3.84E-05	6.88E-16	3.84E-05	4.80E-12	3.84E-05	-4.416	4.57E 05
2.32E-10	2.72E-05	4.86E-16	2.72E-05	1.70E-12	2.72E-05	-4.566	6.47E 05
1.16E-10	1.92E-05	3.44E-16	1.92E-05	6.00E-13	1.92E-05	-4.717	9.15E 05
5.79E-11	1.36E-05	2.43E-16	1.36E-05	2.12E-13	1.36E-05	-4.867	1.29E 06
2.90E-11	9.60E-06	1.72E-16	9.60E-06	7.50E-14	9.60E-06	-5.018	1.83E 06
1.45E-11	6.79E-06	1.22E-16	6.79E-06	2.65E-14	6.79E-06	-5.168	2.59E 06
7.24E-12	4.80E-06	8.60E-17	4.80E-06	9.38E-15	4.80E-06	-5.319	3.66E 06
3.62E-12	3.39E-06	6.08E-17	3.39E-06	3.32E-15	3.39E-06	-5.469	5.17E 06
1.81E-12	2.40E-06	4.30E-17	2.40E-06	1.17E-15	2.40E-06	-5.620	7.32E 06
9.05E-13	1.70E-06	3.04E-17	1.70E-06	4.15E-16	1.70E-06	-5.770	1.03E 07
4.53E-13	1.20E-06	2.15E-17	1.20E-06	1.47E-16	1.20E-06	-5.921	1.46E 07
2.26E-13	8.49E-07	1.52E-17	8.49E-07	5.13E-17	8.49E-07	-6.071	2.07E 07
1.13E-13	6.00E-07	1.07E-17	6.00E-07	1.83E-17	6.00E-07	-6.222	2.93E 07

Table 38. Results of Calculations, t = 150°C, pH = 9.5

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS
TEMPERATURE = 150.0 DEG C PH = 9.5
K1 = 5.52E 00 K2 = 2.70E 02 K3 = 2.00E-09 K4 = 5.70E-11
SOLUBILITY OF I2 IN WATER = 6.22E-02 MOL/L

CONCENTRATIONS IN MOLS/L

CONC I2 IN LIQ	CONC HIO	CONC H2OI+	CONC IODIDE	CONC I3-	TOTAL I2 IN LIQ	LOG TOTAL I	PARTITION COEFF
6.22E-02	2.63E 00	2.38E-11	1.49E-01	2.50E 00	5.21E 00	0.717	4.63E 02
3.11E-02	1.36E 00	1.22E-11	1.45E-01	1.22E 00	2.61E 00	0.417	4.63E 02
1.55E-02	7.16E-01	6.43E-12	1.38E-01	5.78E-01	1.31E 00	0.117	4.65E 02
7.77E-03	3.31E-01	3.51E-12	1.26E-01	2.65E-01	6.64E-01	-0.178	4.71E 02
3.89E-03	2.25E-01	2.02E-12	1.10E-01	1.15E-01	3.44E-01	-0.464	4.88E 02
1.94E-03	1.37E-01	1.23E-12	9.00E-02	4.72E-02	1.86E-01	-0.730	5.29E 02
9.72E-04	8.83E-02	7.92E-13	6.99E-02	1.83E-02	1.08E-01	-0.968	6.11E 02
4.86E-04	5.91E-02	5.30E-13	5.22E-02	6.85E-03	6.64E-02	-1.178	7.54E 02
2.43E-04	4.05E-02	3.64E-13	3.80E-02	2.50E-03	4.33E-02	-1.364	9.83E 02
1.21E-04	2.82E-02	2.53E-13	2.73E-02	8.96E-04	2.92E-02	-1.534	1.33E 03
6.07E-05	1.98E-02	1.78E-13	1.95E-02	3.19E-04	2.02E-02	-1.695	1.83E 03
3.04E-05	1.39E-02	1.25E-13	1.38E-02	1.13E-04	1.41E-02	-1.851	2.56E 03
1.52E-05	9.84E-03	8.83E-14	9.80E-03	4.02E-05	9.89E-03	-2.005	3.60E 03
7.59E-06	6.95E-03	6.24E-14	6.94E-03	1.42E-05	6.97E-03	-2.157	5.07E 03
3.80E-06	4.91E-03	4.41E-14	4.91E-03	5.03E-06	4.92E-03	-2.308	7.16E 03
1.90E-06	3.47E-03	3.12E-14	3.47E-03	1.78E-06	3.48E-03	-2.459	1.01E 04
9.49E-07	2.46E-03	2.20E-14	2.45E-03	6.29E-07	2.46E-03	-2.610	1.43E 04
4.75E-07	1.74E-03	1.56E-14	1.74E-03	2.22E-07	1.74E-03	-2.760	2.02E 04
2.37E-07	1.23E-03	1.10E-14	1.23E-03	7.86E-08	1.23E-03	-2.911	2.86E 04
1.19E-07	8.68E-04	7.79E-15	8.68E-04	2.78E-08	8.68E-04	-3.061	4.04E 04
5.93E-08	6.14E-04	5.51E-15	6.14E-04	9.83E-09	6.14E-04	-3.212	5.71E 04
2.97E-08	4.34E-04	3.90E-15	4.34E-04	3.47E-09	4.34E-04	-3.363	8.08E 04
1.48E-08	3.07E-04	2.75E-15	3.07E-04	1.23E-09	3.07E-04	-3.513	1.14E 05
7.41E-09	2.17E-04	1.95E-15	2.17E-04	4.34E-10	2.17E-04	-3.664	1.62E 05
3.71E-09	1.53E-04	1.38E-15	1.53E-04	1.54E-10	1.53E-04	-3.814	2.28E 05
1.85E-09	1.08E-04	9.74E-16	1.08E-04	5.43E-11	1.08E-04	-3.965	3.23E 05
9.27E-10	7.67E-05	6.89E-16	7.67E-05	1.92E-11	7.67E-05	-4.115	4.57E 05
4.63E-10	5.42E-05	4.87E-16	5.42E-05	6.78E-12	5.42E-05	-4.266	6.46E 05
2.32E-10	3.84E-05	3.44E-16	3.84E-05	2.40E-12	3.84E-05	-4.416	9.14E 05
1.16E-10	2.71E-05	2.43E-16	2.71E-05	8.48E-13	2.71E-05	-4.567	1.29E 06
5.79E-11	1.92E-05	1.72E-16	1.92E-05	3.00E-13	1.92E-05	-4.717	1.83E 06
2.90E-11	1.36E-05	1.22E-16	1.36E-05	1.06E-13	1.36E-05	-4.868	2.58E 06
1.45E-11	9.59E-06	8.61E-17	9.59E-06	3.75E-14	9.59E-06	-5.018	3.66E 06
7.24E-12	6.78E-06	6.09E-17	6.78E-06	1.33E-14	6.78E-06	-5.169	5.17E 06
3.62E-12	4.79E-06	4.30E-17	4.79E-06	4.69E-15	4.79E-06	-5.319	7.31E 06
1.81E-12	3.39E-06	3.04E-17	3.39E-06	1.66E-15	3.39E-06	-5.470	1.03E 07
9.05E-13	2.40E-06	2.15E-17	2.40E-06	5.86E-16	2.40E-06	-5.620	1.46E 07
4.53E-13	1.70E-06	1.52E-17	1.70E-06	2.07E-16	1.70E-06	-5.771	2.07E 07
2.26E-13	1.20E-06	1.08E-17	1.20E-06	7.32E-17	1.20E-06	-5.921	2.92E 07
1.13E-13	8.48E-07	7.61E-18	8.48E-07	2.59E-17	8.48E-07	-6.072	4.14E 07

Table 39. Results Including Iodate Reaction, t = 25°C, pH = 7.0

CALCULATION OF PARTITION COEFFICIENT FOR IODINE BETWEEN WATER AND AIR, ASSUMING EQUILIBRIUM IODATE FORMATION

TEMPERATURE = 25.0 DEG C PH = 7.0 SATURATION CONC OF I2 IN LIQUID = 1.320D-03 MOL/L

K1 = 7.46D 01 K2 = 7.58D 02 K3 = 5.40D-13

K4 = 1.20D-11 K5 = 4.00D-48

CONCENTRATIONS IN MOLS/L

CONC OF I2	CONC OF HIO	CONC OF H2OI+	CONC OF I-	CONC OF I3-	CONC OF IO3-	TOTAL I2 (AQ)	LOG C(I2)	PART COEFF
1.320D-03	1.337D-06	2.962D-12	5.348D-03	5.349D-03	2.139D-03	1.309D-02	-1.883	7.396D 02
6.600D-04	9.009D-07	1.996D-12	3.968D-03	1.984D-03	1.190D-03	6.215D-03	-2.207	7.025D 02
3.300D-04	6.179D-07	1.369D-12	2.892D-03	7.231D-04	7.229D-04	3.222D-03	-2.492	7.285D 02
1.650D-04	4.293D-07	9.514D-13	2.081D-03	2.602D-04	4.662D-04	1.830D-03	-2.738	8.275D 02
8.250D-05	3.007D-07	6.663D-13	1.486D-03	9.286D-05	3.157D-04	1.123D-03	-2.950	1.015D 03
4.125D-05	2.116D-07	4.688D-13	1.056D-03	3.300D-05	2.177D-04	7.276D-04	-3.138	1.316D 03
2.062D-05	1.492D-07	3.307D-13	7.485D-04	1.170D-05	1.520D-04	4.885D-04	-3.311	1.767D 03
1.031D-05	1.054D-07	2.335D-13	5.299D-04	4.140D-06	1.068D-04	3.349D-04	-3.475	2.423D 03
5.156D-06	7.447D-08	1.650D-13	3.750D-04	1.465D-06	7.527D-05	2.325D-04	-3.634	3.364D 03
2.578D-06	5.264D-08	1.166D-13	2.652D-04	5.180D-07	5.314D-05	1.626D-04	-3.789	4.704D 03
1.289D-06	3.722D-08	8.247D-14	1.876D-04	1.832D-07	3.754D-05	1.141D-04	-3.943	6.606D 03
6.445D-07	2.631D-08	5.831D-14	1.326D-04	6.477D-08	2.654D-05	8.035D-05	-4.095	9.300D 03
3.223D-07	1.861D-08	4.123D-14	9.380D-05	2.290D-08	1.876D-05	5.665D-05	-4.247	1.311D 04
1.611D-07	1.316D-08	2.915D-14	6.633D-05	8.097D-09	1.326D-05	3.998D-05	-4.398	1.851D 04
8.057D-08	9.303D-09	2.061D-14	4.690D-05	2.863D-09	9.379D-06	2.823D-05	-4.549	2.614D 04
4.028D-08	6.578D-09	1.458D-14	3.316D-05	1.012D-09	6.632D-06	1.994D-05	-4.700	3.693D 04
2.014D-08	4.651D-09	1.031D-14	2.345D-05	3.578D-10	4.689D-06	1.409D-05	-4.851	5.220D 04
1.007D-08	3.289D-09	7.288D-15	1.658D-05	1.265D-10	3.316D-06	9.961D-06	-5.002	7.379D 04
5.035D-09	2.326D-09	5.153D-15	1.173D-05	4.473D-11	2.345D-06	7.041D-06	-5.152	1.043D 05
2.518D-09	1.645D-09	3.644D-15	8.291D-06	1.581D-11	1.658D-06	4.978D-06	-5.303	1.475D 05
1.259D-09	1.163D-09	2.577D-15	5.863D-06	5.591D-12	1.172D-06	3.519D-06	-5.454	2.086D 05
6.294D-10	8.223D-10	1.822D-15	4.146D-06	1.977D-12	8.289D-07	2.488D-06	-5.604	2.949D 05
3.147D-10	5.814D-10	1.288D-15	2.931D-06	6.989D-13	5.861D-07	1.759D-06	-5.755	4.170D 05
1.574D-10	4.111D-10	9.110D-16	2.073D-06	2.471D-13	4.145D-07	1.244D-06	-5.905	5.898D 05
7.868D-11	2.907D-10	6.442D-16	1.466D-06	8.736D-14	2.931D-07	8.796D-07	-6.056	8.340D 05
3.934D-11	2.056D-10	4.555D-16	1.036D-06	3.089D-14	2.072D-07	6.220D-07	-6.206	1.179D 06
1.967D-11	1.454D-10	3.221D-16	7.328D-07	1.092D-14	1.465D-07	4.398D-07	-6.357	1.668D 06
9.835D-12	1.028D-10	2.277D-16	5.182D-07	3.861D-15	1.036D-07	3.110D-07	-6.507	2.359D 06
4.917D-12	7.268D-11	1.610D-16	3.664D-07	1.365D-15	7.327D-08	2.199D-07	-6.658	3.336D 06
2.459D-12	5.139D-11	1.139D-16	2.591D-07	4.826D-16	5.181D-08	1.555D-07	-6.808	4.718D 06
1.229D-12	3.634D-11	8.052D-17	1.832D-07	1.706D-16	3.663D-08	1.099D-07	-6.959	6.671D 06
6.147D-13	2.570D-11	5.694D-17	1.295D-07	6.033D-17	2.590D-08	7.774D-08	-7.109	9.435D 06
3.073D-13	1.817D-11	4.026D-17	9.160D-08	2.133D-17	1.832D-08	5.497D-08	-7.260	1.334D 07
1.537D-13	1.285D-11	2.847D-17	6.477D-08	7.541D-18	1.295D-08	3.887D-08	-7.410	1.887D 07
7.683D-14	9.085D-12	2.013D-17	4.580D-08	2.666D-18	9.159D-09	2.748D-08	-7.561	2.669D 07
3.842D-14	6.424D-12	1.423D-17	3.239D-08	9.426D-19	6.476D-09	1.943D-08	-7.711	3.774D 07
1.921D-14	4.542D-12	1.007D-17	2.290D-08	3.333D-19	4.579D-09	1.374D-08	-7.862	5.337D 07
9.604D-15	3.212D-12	7.117D-18	1.619D-08	1.178D-19	3.238D-09	9.717D-09	-8.012	7.548D 07
4.802D-15	2.271D-12	5.033D-18	1.145D-08	4.166D-20	2.290D-09	6.871D-09	-8.163	1.067D 08
2.401D-15	1.606D-12	3.559D-18	8.097D-09	1.473D-20	1.619D-09	4.859D-09	-8.313	1.510D 08

Table 40. Results Including Iodate Reaction, t = 25°C, pH = 9.0

CALCULATION OF PARTITION COEFFICIENT FOR IODINE BETWEEN WATER AND AIR, ASSUMING EQUILIBRIUM IODATE FORMATION

TEMPERATURE = 25.0 DEG C PH = 9.0 SATURATION CONC OF I2 IN LIQUID = 1.320D-03 MOL/L

K1 = 7.46D 01 K2 = 7.58D 02 K3 = 5.40D-13

K4 = 1.20D-11 K5 = 4.00D-48

CONCENTRATIONS IN MOLS/L

CONC OF I2	CONC OF HIO	CONC OF H2OI+	CONC OF I-	CONC OF I3-	CONC OF IO3-	TOTAL I2 (AQ)	LOG C(I2)	PART COEFF
1.320D-03	1.337D-06	2.959D-14	5.353D-01	5.353D-01	2.141D-01	1.179D 00	0.071	6.663D 04
6.600D-04	9.009D-07	1.995D-14	3.971D-01	1.985D-01	1.191D-01	5.566D-01	-0.254	6.291D 04
3.300D-04	6.180D-07	1.368D-14	2.894D-01	7.236D-02	7.236D-02	2.898D-01	-0.538	6.551D 04
1.650D-04	4.294D-07	9.506D-15	2.083D-01	2.604D-02	4.687D-02	1.668D-01	-0.778	7.541D 04
8.250D-05	3.007D-07	6.658D-15	1.487D-01	9.294D-03	3.160D-02	1.042D-01	-0.982	9.419D 04
4.125D-05	2.116D-07	4.685D-15	1.057D-01	3.302D-03	2.179D-02	6.872D-02	-1.163	1.243D 05
2.062D-05	1.492D-07	3.304D-15	7.491D-02	1.170D-03	1.522D-02	4.684D-02	-1.329	1.694D 05
1.031D-05	1.054D-07	2.333D-15	5.304D-02	4.144D-04	1.069D-02	3.250D-02	-1.488	2.351D 05
5.156D-06	7.447D-08	1.649D-15	3.753D-02	1.466D-04	7.535D-03	2.276D-02	-1.643	3.292D 05
2.578D-06	5.264D-08	1.166D-15	2.654D-02	5.185D-05	5.319D-03	1.601D-02	-1.796	4.633D 05
1.289D-06	3.722D-08	8.240D-16	1.877D-02	1.833D-05	3.758D-03	1.129D-02	-1.947	6.536D 05
6.445D-07	2.632D-08	5.826D-16	1.328D-02	6.482D-06	2.656D-03	7.976D-03	-2.098	9.232D 05
3.223D-07	1.861D-08	4.120D-16	9.387D-03	2.292D-06	1.878D-03	5.636D-03	-2.249	1.305D 06
1.611D-07	1.316D-08	2.913D-16	6.638D-03	8.103D-07	1.328D-03	3.984D-03	-2.400	1.845D 06
8.057D-08	9.303D-09	2.060D-16	4.694D-03	2.865D-07	9.388D-04	2.817D-03	-2.550	2.608D 06
4.028D-08	6.578D-09	1.456D-16	3.319D-03	1.013D-07	6.638D-04	1.992D-03	-2.701	3.688D 06
2.014D-08	4.652D-09	1.030D-16	2.347D-03	3.581D-08	4.694D-04	1.408D-03	-2.851	5.216D 06
1.007D-08	3.289D-09	7.282D-17	1.660D-03	1.266D-08	3.319D-04	9.958D-04	-3.002	7.376D 06
5.035D-09	2.326D-09	5.149D-17	1.173D-03	4.477D-09	2.347D-04	7.041D-04	-3.152	1.043D 07
2.518D-09	1.645D-09	3.641D-17	8.298D-04	1.583D-09	1.660D-04	4.979D-04	-3.303	1.475D 07
1.259D-09	1.163D-09	2.575D-17	5.867D-04	5.596D-10	1.173D-04	3.520D-04	-3.453	2.086D 07
6.294D-10	8.223D-10	1.821D-17	4.149D-04	1.978D-10	8.298D-05	2.489D-04	-3.604	2.950D 07
3.147D-10	5.815D-10	1.287D-17	2.934D-04	6.995D-11	5.867D-05	1.760D-04	-3.754	4.172D 07
1.574D-10	4.111D-10	9.103D-18	2.074D-04	2.473D-11	4.149D-05	1.245D-04	-3.905	5.901D 07
7.868D-11	2.907D-10	6.437D-18	1.467D-04	8.743D-12	2.934D-05	8.801D-05	-4.055	8.345D 07
3.934D-11	2.056D-10	4.551D-18	1.037D-04	3.091D-12	2.074D-05	6.223D-05	-4.206	1.180D 08
1.967D-11	1.454D-10	3.218D-18	7.334D-05	1.093D-12	1.467D-05	4.401D-05	-4.356	1.669D 08
9.835D-12	1.028D-10	2.276D-18	5.186D-05	3.864D-13	1.037D-05	3.112D-05	-4.507	2.360D 08
4.917D-12	7.268D-11	1.609D-18	3.667D-05	1.366D-13	7.334D-06	2.200D-05	-4.658	3.338D 08
2.459D-12	5.139D-11	1.138D-18	2.593D-05	4.830D-14	5.186D-06	1.556D-05	-4.808	4.721D 08
1.229D-12	3.634D-11	8.046D-19	1.834D-05	1.708D-14	3.667D-06	1.100D-05	-4.959	6.676D 08
6.147D-13	2.570D-11	5.689D-19	1.297D-05	6.038D-15	2.593D-06	7.779D-06	-5.109	9.441D 08
3.073D-13	1.817D-11	4.023D-19	9.168D-06	2.135D-15	1.834D-06	5.501D-06	-5.260	1.335D 09
1.537D-13	1.285D-11	2.845D-19	6.483D-06	7.547D-16	1.297D-06	3.890D-06	-5.410	1.888D 09
7.683D-14	9.085D-12	2.011D-19	4.584D-06	2.668D-16	9.168D-07	2.750D-06	-5.561	2.670D 09
3.842D-14	6.424D-12	1.422D-19	3.241D-06	9.434D-17	6.483D-07	1.945D-06	-5.711	3.776D 09
1.921D-14	4.543D-12	1.006D-19	2.292D-06	3.335D-17	4.584D-07	1.375D-06	-5.862	5.341D 09
9.604D-15	3.212D-12	7.111D-20	1.621D-06	1.179D-17	3.241D-07	9.724D-07	-6.012	7.553D 09
4.802D-15	2.271D-12	5.029D-20	1.146D-06	4.169D-18	2.292D-07	6.876D-07	-6.163	1.068D 10
2.401D-15	1.606D-12	3.556D-20	8.103D-07	1.474D-18	1.621D-07	4.862D-07	-6.313	1.511D 10

Table 41. Results Including Iodate Reaction, t = 100°C, pH = 7.0

CALCULATION OF PARTITION COEFFICIENT FOR IODINE BETWEEN WATER AND AIR, ASSUMING EQUILIBRIUM IODATE FORMATION

TEMPERATURE = 100.0 DEG C PH = 7.0 SATURATION CONC OF I2 IN LIQUID = 1.750D-02 MOL/L

K1 = 9.00D 00 K2 = 2.98D 02 K3 = 1.50D-10

K4 = 3.90D-11 K5 = 1.03D-36

CONCENTRATIONS IN MOLS/L

CONC OF I2	CONC OF HIO	CONC OF H2OI+	CONC OF I-	CONC OF I3-	CONC OF IO3-	TOTAL I2 (AQ)	LOG C(I2)	PART COEFF
1.750D-02	2.047D-05	5.306D-13	1.286D 00	6.704D 00	1.598D 00	1.151D 01	1.061	5.922D 03
8.750D-03	1.322D-05	3.427D-13	9.959D-01	2.595D 00	7.182D-01	4.758D 00	0.677	4.894D 03
4.375D-03	8.673D-06	2.249D-13	7.588D-01	9.886D-01	3.495D-01	2.041D 00	0.310	4.200D 03
2.187D-03	5.802D-06	1.504D-13	5.671D-01	3.695D-01	1.873D-01	9.336D-01	-0.030	3.841D 03
1.094D-03	3.955D-06	1.025D-13	4.160D-01	1.355D-01	1.103D-01	4.675D-01	-0.330	3.847D 03
5.469D-04	2.736D-06	7.094D-14	3.006D-01	4.896D-02	6.992D-02	2.593D-01	-0.586	4.267D 03
2.734D-04	1.912D-06	4.956D-14	2.152D-01	1.752D-02	4.654D-02	1.574D-01	-0.803	5.181D 03
1.367D-04	1.343D-06	3.482D-14	1.531D-01	6.234D-03	3.187D-02	1.020D-01	-0.991	6.714D 03
6.836D-05	9.466D-07	2.454D-14	1.086D-01	2.212D-03	2.217D-02	6.879D-02	-1.162	9.057D 03
3.418D-05	6.682D-07	1.732D-14	7.695D-02	7.832D-04	1.555D-02	4.745D-02	-1.324	1.250D 04
1.709D-05	4.721D-07	1.224D-14	5.445D-02	2.771D-04	1.095D-02	3.313D-02	-1.480	1.745D 04
8.545D-06	3.337D-07	8.651D-15	3.852D-02	9.802D-05	7.724D-03	2.328D-02	-1.633	2.452D 04
4.272D-06	2.359D-07	6.116D-15	2.724D-02	3.466D-05	5.456D-03	1.641D-02	-1.785	3.456D 04
2.136D-06	1.668D-07	4.324D-15	1.927D-02	1.226D-05	3.856D-03	1.158D-02	-1.936	4.879D 04
1.068D-06	1.179D-07	3.057D-15	1.362D-02	4.334D-06	2.726D-03	8.183D-03	-2.087	6.895D 04
5.341D-07	8.339D-08	2.162D-15	9.634D-03	1.532D-06	1.927D-03	5.784D-03	-2.238	9.746D 04
2.670D-07	5.897D-08	1.529D-15	6.812D-03	5.417D-07	1.363D-03	4.089D-03	-2.388	1.378D 05
1.335D-07	4.169D-08	1.081D-15	4.817D-03	1.915D-07	9.635D-04	2.891D-03	-2.539	1.949D 05
6.676D-08	2.948D-08	7.643D-16	3.406D-03	6.772D-08	6.813D-04	2.044D-03	-2.690	2.756D 05
3.338D-08	2.085D-08	5.405D-16	2.409D-03	2.394D-08	4.817D-04	1.445D-03	-2.840	3.897D 05
1.669D-08	1.474D-08	3.822D-16	1.703D-03	8.465D-09	3.406D-04	1.022D-03	-2.991	5.511D 05
8.345D-09	1.042D-08	2.702D-16	1.204D-03	2.993D-09	2.409D-04	7.226D-04	-3.141	7.793D 05
4.172D-09	7.371D-09	1.911D-16	8.516D-04	1.058D-09	1.703D-04	5.110D-04	-3.292	1.102D 06
2.086D-09	5.212D-09	1.351D-16	6.022D-04	3.741D-10	1.204D-04	3.613D-04	-3.442	1.559D 06
1.043D-09	3.685D-09	9.554D-17	4.258D-04	1.323D-10	8.516D-05	2.555D-04	-3.593	2.204D 06
5.215D-10	2.606D-09	6.756D-17	3.011D-04	4.676D-11	6.021D-05	1.806D-04	-3.743	3.117D 06
2.608D-10	1.843D-09	4.777D-17	2.129D-04	1.653D-11	4.258D-05	1.277D-04	-3.894	4.409D 06
1.304D-10	1.303D-09	3.378D-17	1.505D-04	5.845D-12	3.011D-05	9.032D-05	-4.044	6.235D 06
6.519D-11	9.213D-10	2.389D-17	1.064D-04	2.067D-12	2.129D-05	6.387D-05	-4.195	8.817D 06
3.260D-11	6.515D-10	1.689D-17	7.527D-05	7.306D-13	1.505D-05	4.516D-05	-4.345	1.247D 07
1.630D-11	4.607D-10	1.194D-17	5.322D-05	2.583D-13	1.064D-05	3.193D-05	-4.496	1.763D 07
8.149D-12	3.257D-10	8.445D-18	3.763D-05	9.133D-14	7.527D-06	2.258D-05	-4.646	2.494D 07
4.075D-12	2.303D-10	5.971D-18	2.661D-05	3.229D-14	5.322D-06	1.597D-05	-4.797	3.527D 07
2.037D-12	1.629D-10	4.222D-18	1.882D-05	1.142D-14	3.763D-06	1.129D-05	-4.947	4.988D 07
1.019D-12	1.152D-10	2.986D-18	1.331D-05	4.036D-15	2.661D-06	7.983D-06	-5.098	7.054D 07
5.093D-13	8.144D-11	2.111D-18	9.409D-06	1.427D-15	1.882D-06	5.645D-06	-5.248	9.975D 07
2.547D-13	5.758D-11	1.493D-18	6.653D-06	5.045D-16	1.331D-06	3.992D-06	-5.399	1.411D 08
1.273D-13	4.072D-11	1.056D-18	4.704D-06	1.784D-16	9.409D-07	2.823D-06	-5.549	1.995D 08
6.366D-14	2.879D-11	7.464D-19	3.326D-06	6.307D-17	6.653D-07	1.996D-06	-5.700	2.821D 08
3.183D-14	2.036D-11	5.278D-19	2.352D-06	2.230D-17	4.704D-07	1.411D-06	-5.850	3.990D 08

Table 42. Results Including Iodate Reaction, t = 100°C, pH = 9.0

CALCULATION OF PARTITION COEFFICIENT FOR IODINE BETWEEN WATER AND AIR, ASSUMING EQUILIBRIUM IODATE FORMATION

TEMPERATURE = 100.0 DEG C PH = 9.0 SATURATION CONC OF I2 IN LIQUID = 1.750D-02 MOL/L

K1 = 9.00D 00 K2 = 2.98D 02 K3 = 1.50D-10

K4 = 3.90D-11 K5 = 1.03D-36

CONCENTRATIONS IN MOLS/L

CONC OF I2	CONC OF HIO	CONC OF H2OI+	CONC OF I-	CONC OF I3-	CONC OF IO3-	TOTAL I2 (AQ)	LOG C(I2)	PART COEFF
4.375D-03	8.673D-06	2.247D-15	7.595D 01	9.895D 01	3.498D 01	2.039D 02	2.309	4.194D 05
2.187D-03	5.802D-06	1.503D-15	5.676D 01	3.698D 01	1.875D 01	9.322D 01	1.970	3.835D 05
1.094D-03	3.955D-06	1.025D-15	4.163D 01	1.356D 01	1.104D 01	4.668D 01	1.669	3.841D 05
5.469D-04	2.736D-06	7.088D-16	3.009D 01	4.900D 00	6.998D 00	2.589D 01	1.413	4.262D 05
2.734D-04	1.912D-06	4.952D-16	2.154D 01	1.754D 00	4.658D 00	1.573D 01	1.197	5.177D 05
1.367D-04	1.343D-06	3.479D-16	1.533D 01	6.240D-01	3.190D 00	1.019D 01	1.008	6.710D 05
6.836D-05	9.466D-07	2.452D-16	1.087D 01	2.213D-01	2.219D 00	6.878D 00	0.837	9.055D 05
3.418D-05	6.682D-07	1.731D-16	7.701D 00	7.838D-02	1.556D 00	4.746D 00	0.676	1.250D 06
1.709D-05	4.721D-07	1.223D-16	5.450D 00	2.774D-02	1.096D 00	3.314D 00	0.520	1.745D 06
8.545D-06	3.337D-07	8.644D-17	3.855D 00	9.810D-03	7.730D-01	2.329D 00	0.367	2.453D 06
4.272D-06	2.359D-07	6.111D-17	2.727D 00	3.469D-03	5.460D-01	1.642D 00	0.215	3.458D 06
2.136D-06	1.668D-07	4.321D-17	1.928D 00	1.227D-03	3.859D-01	1.159D 00	0.064	4.883D 06
1.068D-06	1.179D-07	3.055D-17	1.364D 00	4.337D-04	2.728D-01	8.188D-01	-0.087	6.900D 06
5.341D-07	8.339D-08	2.160D-17	9.642D-01	1.533D-04	1.929D-01	5.788D-01	-0.237	9.754D 06
2.670D-07	5.897D-08	1.527D-17	6.818D-01	5.422D-05	1.364D-01	4.092D-01	-0.388	1.379D 07
1.335D-07	4.170D-08	1.080D-17	4.821D-01	1.917D-05	9.643D-02	2.893D-01	-0.539	1.950D 07
6.676D-08	2.948D-08	7.637D-18	3.409D-01	6.777D-06	6.818D-02	2.046D-01	-0.689	2.758D 07
3.338D-08	2.085D-08	5.400D-18	2.411D-01	2.396D-06	4.821D-02	1.446D-01	-0.840	3.900D 07
1.669D-08	1.474D-08	3.818D-18	1.705D-01	8.472D-07	3.409D-02	1.023D-01	-0.990	5.515D 07
8.345D-09	1.042D-08	2.700D-18	1.205D-01	2.995D-07	2.411D-02	7.232D-02	-1.141	7.800D 07
4.172D-09	7.371D-09	1.909D-18	8.523D-02	1.059D-07	1.705D-02	5.114D-02	-1.291	1.103D 08
2.086D-09	5.212D-09	1.350D-18	6.026D-02	3.744D-08	1.205D-02	3.616D-02	-1.442	1.560D 08
1.043D-09	3.685D-09	9.546D-19	4.261D-02	1.324D-08	8.523D-03	2.557D-02	-1.592	2.206D 08
5.215D-10	2.606D-09	6.750D-19	3.013D-02	4.680D-09	6.027D-03	1.808D-02	-1.743	3.120D 08
2.608D-10	1.843D-09	4.773D-19	2.131D-02	1.655D-09	4.261D-03	1.278D-02	-1.893	4.412D 08
1.304D-10	1.303D-09	3.375D-19	1.507D-02	5.850D-10	3.013D-03	9.040D-03	-2.044	6.240D 08
6.519D-11	9.213D-10	2.387D-19	1.065D-02	2.068D-10	2.131D-03	6.392D-03	-2.194	8.824D 08
3.260D-11	6.515D-10	1.688D-19	7.533D-03	7.312D-11	1.507D-03	4.520D-03	-2.345	1.248D 09
1.630D-11	4.607D-10	1.193D-19	5.327D-03	2.585D-11	1.065D-03	3.196D-03	-2.495	1.765D 09
8.149D-12	3.257D-10	8.438D-20	3.767D-03	9.141D-12	7.533D-04	2.260D-03	-2.646	2.496D 09
4.075D-12	2.303D-10	5.966D-20	2.663D-03	3.232D-12	5.327D-04	1.598D-03	-2.796	3.530D 09
2.037D-12	1.629D-10	4.219D-20	1.883D-03	1.143D-12	3.767D-04	1.130D-03	-2.947	4.992D 09
1.019D-12	1.152D-10	2.983D-20	1.332D-03	4.040D-13	2.663D-04	7.990D-04	-3.097	7.060D 09
5.093D-13	8.144D-11	2.109D-20	9.416D-04	1.428D-13	1.883D-04	5.650D-04	-3.248	9.984D 09
2.547D-13	5.758D-11	1.492D-20	6.658D-04	5.049D-14	1.332D-04	3.995D-04	-3.398	1.412D 10
1.273D-13	4.072D-11	1.055D-20	4.708D-04	1.785D-14	9.416D-05	2.825D-04	-3.549	1.997D 10
6.366D-14	2.879D-11	7.458D-21	3.329D-04	6.312D-15	6.658D-05	1.998D-04	-3.700	2.824D 10
3.183D-14	2.036D-11	5.274D-21	2.354D-04	2.232D-15	4.708D-05	1.412D-04	-3.850	3.993D 10
1.592D-14	1.440D-11	3.729D-21	1.665D-04	7.890D-16	3.329D-05	9.988D-05	-4.001	5.648D 10
7.958D-15	1.018D-11	2.637D-21	1.177D-04	2.789D-16	2.354D-05	7.062D-05	-4.151	7.987D 10

IHC002I STOP 0

Table 43. Results Including Effect of HIO Volatility, t = 25°C, pH = 7.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS, INCLUDING EFFECT OF HOI VOLATILITY

TEMPERATURE = 25.0 DEG C PH =7.0
K1 =7.46E 01 K2 =7.58E 02 K3 =5.40E-13
K4 =1.20E-11 K5 =7.18E 02
RATIO OF GAS VOLUME TO LIQUID VOLUME =1.00E 02

CONCENTRATIONS IN MOLS/L

CONC OF I2 IN GAS	CONC OF I2 IN LIQUID	CONC HIO IN LIQUID	CONC OF H2/I+ (AQ)	CONC OF I-	CONC OF I3-	CONC OF HIO IN GAS	TOTAL I IN LIQUID	TOTAL I IN GAS	LOG TOTAL I (AQ)	PARTITION COEFFICIENT
1.77E-05	1.32E-03	1.12E-04	2.48E-10	6.38E-05	6.38E-05	1.56E-07	1.50E-03	1.78E-05	-2.823	8.46E 01
8.85E-06	6.60E-04	6.86E-05	1.52E-10	5.21E-05	2.61E-05	9.55E-08	7.59E-04	8.89E-06	-3.120	8.54E 01
4.42E-06	3.30E-04	4.43E-05	9.81E-11	4.04E-05	1.01E-05	6.17E-08	3.87E-04	4.45E-06	-3.412	8.70E 01
2.21E-06	1.65E-04	2.97E-05	6.58E-11	3.01E-05	3.76E-06	4.14E-08	2.01E-04	2.23E-06	-3.698	8.98E 01
1.11E-06	8.25E-05	2.04E-05	4.52E-11	2.19E-05	1.37E-06	2.84E-08	1.06E-04	1.12E-06	-3.976	9.44E 01
5.53E-07	4.12E-05	1.42E-05	3.15E-11	1.57E-05	4.91E-07	1.98E-08	5.70E-05	5.63E-07	-4.244	1.01E 02
2.76E-07	2.06E-05	9.98E-06	2.21E-11	1.12E-05	1.75E-07	1.39E-08	3.15E-05	2.83E-07	-4.502	1.11E 02
1.38E-07	1.03E-05	7.03E-06	1.56E-11	7.95E-06	6.21E-08	9.79E-09	1.79E-05	1.43E-07	-4.747	1.25E 02
6.91E-08	5.16E-06	4.96E-06	1.10E-11	5.63E-06	2.20E-08	6.91E-09	1.05E-05	7.26E-08	-4.979	1.44E 02
3.46E-08	2.58E-06	3.50E-06	7.76E-12	3.98E-06	7.78E-09	4.88E-09	6.33E-06	3.70E-08	-5.198	1.71E 02
1.73E-08	1.29E-06	2.48E-06	5.49E-12	2.82E-06	2.75E-09	3.45E-09	3.94E-06	1.90E-08	-5.404	2.07E 02
8.64E-09	6.45E-07	1.75E-06	3.88E-12	1.99E-06	9.73E-10	2.44E-09	2.52E-06	9.86E-09	-5.599	2.55E 02
4.32E-09	3.22E-07	1.24E-06	2.74E-12	1.41E-06	3.44E-10	1.72E-09	1.65E-06	5.18E-09	-5.783	3.18E 02
2.16E-09	1.61E-07	8.75E-07	1.94E-12	9.97E-07	1.22E-10	1.22E-09	1.10E-06	2.77E-09	-5.960	3.96E 02
1.08E-09	8.06E-08	6.19E-07	1.37E-12	7.05E-07	4.30E-11	8.62E-10	7.43E-07	1.51E-09	-6.129	4.91E 02
5.40E-10	4.03E-08	4.38E-07	9.70E-13	4.99E-07	1.52E-11	6.09E-10	5.08E-07	8.45E-10	-6.294	6.02E 02
2.70E-10	2.01E-08	3.09E-07	6.86E-13	3.53E-07	5.38E-12	4.31E-10	3.51E-07	4.85E-10	-6.455	7.23E 02
1.35E-10	1.01E-08	2.19E-07	4.85E-13	2.49E-07	1.90E-12	3.05E-10	2.44E-07	2.87E-10	-6.612	8.49E 02
6.75E-11	5.04E-09	1.55E-07	3.43E-13	1.76E-07	6.72E-13	2.15E-10	1.71E-07	1.75E-10	-6.768	9.73E 02
3.37E-11	2.52E-09	1.09E-07	2.42E-13	1.25E-07	2.38E-13	1.52E-10	1.20E-07	1.10E-10	-6.923	1.09E 03
1.69E-11	1.26E-09	7.74E-08	1.71E-13	8.81E-08	8.40E-14	1.08E-10	8.40E-08	7.07E-11	-7.076	1.19E 03
8.44E-12	6.29E-10	5.47E-08	1.21E-13	6.23E-08	2.97E-14	7.62E-11	5.91E-08	4.65E-11	-7.228	1.27E 03
4.22E-12	3.15E-10	3.87E-08	8.57E-14	4.41E-08	1.05E-14	5.39E-11	4.17E-08	3.12E-11	-7.380	1.34E 03
2.11E-12	1.57E-10	2.73E-08	6.06E-14	3.12E-08	3.71E-15	3.81E-11	2.94E-08	2.12E-11	-7.531	1.39E 03
1.05E-12	7.87E-11	1.93E-08	4.29E-14	2.20E-08	1.31E-15	2.69E-11	2.08E-08	1.45E-11	-7.683	1.43E 03
5.27E-13	3.93E-11	1.37E-08	3.03E-14	1.56E-08	4.64E-16	1.90E-11	1.47E-08	1.01E-11	-7.834	1.46E 03
2.64E-13	1.97E-11	9.67E-09	2.14E-14	1.10E-08	1.64E-16	1.35E-11	1.04E-08	7.00E-12	-7.985	1.48E 03
1.32E-13	9.83E-12	6.84E-09	1.52E-14	7.79E-09	5.80E-17	9.52E-12	7.32E-09	4.89E-12	-8.135	1.50E 03
6.59E-14	4.92E-12	4.83E-09	1.07E-14	5.51E-09	2.05E-17	6.73E-12	5.18E-09	3.43E-12	-8.286	1.51E 03
3.30E-14	2.46E-12	3.42E-09	7.58E-15	3.89E-09	7.25E-18	4.76E-12	3.66E-09	2.41E-12	-8.437	1.52E 03
1.65E-14	1.23E-12	2.42E-09	5.36E-15	2.75E-09	2.56E-18	3.37E-12	2.59E-09	1.70E-12	-8.587	1.52E 03
8.24E-15	6.15E-13	1.71E-09	3.79E-15	1.95E-09	9.07E-19	2.38E-12	1.83E-09	1.20E-12	-8.738	1.53E 03
4.12E-15	3.07E-13	1.21E-09	2.68E-15	1.38E-09	3.21E-19	1.68E-12	1.29E-09	8.46E-13	-8.888	1.53E 03
2.06E-15	1.54E-13	8.55E-10	1.89E-15	9.74E-10	1.13E-19	1.19E-12	9.14E-10	5.97E-13	-9.039	1.53E 03

Table 44. Results Including Effect of HIO Volatility, t = 25°C, pH = 9.0

RESULTS OF IODINE-WATER PARTITION COEFFICIENT CALCULATIONS, INCLUDING EFFECT OF HOI VOLATILITY

TEMPERATURE = 25.0 DEG C PH =9.0
K1 =7.46E 01 K2 =7.58E 02 K3 =5.40E-13
K4 =1.20E-11 K5 =7.18E 02
RATIO OF GAS VOLUME TO LIQUID VOLUME =1.00E 02

CONCENTRATIONS IN MOLS/L

CONC OF I2 IN GAS	CONC OF I2 IN LIQUID	CONC HIO IN LIQUID	CONC OF H2/I+ (AQ)	CONC OF I-	CONC OF I3-	CONC OF HIO IN GAS	TOTAL I IN LIQUID	TOTAL I IN GAS	LOG TOTAL I (AQ)	PARTITION COEFFICIENT
1.77E-05	1.32E-03	1.12E-03	2.48E-11	6.38E-04	6.38E-04	1.56E-06	3.16E-03	1.85E-05	-2.501	1.71E 02
8.85E-06	6.60E-04	6.86E-04	1.52E-11	5.21E-04	2.61E-04	9.56E-07	1.65E-03	9.33E-06	-2.781	1.77E 02
4.42E-06	3.30E-04	4.43E-04	9.81E-12	4.04E-04	1.01E-04	6.17E-07	9.05E-04	4.73E-06	-3.043	1.91E 02
2.21E-06	1.65E-04	2.97E-04	6.58E-12	3.01E-04	3.76E-05	4.14E-07	5.20E-04	2.42E-06	-3.284	2.15E 02
1.11E-06	8.25E-05	2.04E-04	4.52E-12	2.19E-04	1.37E-05	2.84E-07	3.15E-04	1.25E-06	-3.502	2.52E 02
5.53E-07	4.12E-05	1.42E-04	3.15E-12	1.57E-04	4.91E-06	1.98E-07	1.98E-04	6.52E-07	-3.703	3.04E 02
2.76E-07	2.06E-05	9.98E-05	2.21E-12	1.12E-04	1.75E-06	1.39E-07	1.29E-04	3.46E-07	-3.889	3.73E 02
1.38E-07	1.03E-05	7.03E-05	1.56E-12	7.95E-05	6.21E-07	9.79E-08	8.61E-05	1.87E-07	-4.065	4.60E 02
6.91E-08	5.16E-06	4.96E-05	1.10E-12	5.63E-05	2.20E-07	6.91E-08	5.85E-05	1.04E-07	-4.233	5.64E 02
3.46E-08	2.58E-06	3.51E-05	7.76E-13	3.99E-05	7.79E-08	4.88E-08	4.02E-05	5.90E-08	-4.396	6.81E 02
1.73E-08	1.29E-06	2.48E-05	5.49E-13	2.82E-05	2.75E-08	3.45E-08	2.78E-05	3.45E-08	-4.556	8.06E 02
8.64E-09	6.45E-07	1.75E-05	3.88E-13	1.99E-05	9.74E-09	2.44E-08	1.94E-05	2.08E-08	-4.712	9.31E 02
4.32E-09	3.22E-07	1.24E-05	2.74E-13	1.41E-05	3.44E-09	1.72E-08	1.36E-05	1.29E-08	-4.867	1.05E 03
2.16E-09	1.61E-07	8.76E-06	1.94E-13	9.97E-06	1.22E-09	1.22E-08	9.53E-06	8.26E-09	-5.021	1.15E 03
1.08E-09	8.06E-08	6.19E-06	1.37E-13	7.05E-06	4.30E-10	8.62E-09	6.70E-06	5.39E-09	-5.174	1.24E 03
5.40E-10	4.03E-08	4.38E-06	9.69E-14	4.99E-06	1.52E-10	6.10E-09	4.72E-06	3.59E-09	-5.326	1.32E 03
2.70E-10	2.01E-08	3.10E-06	6.85E-14	3.53E-06	5.38E-11	4.31E-09	3.33E-06	2.43E-09	-5.477	1.37E 03
1.35E-10	1.01E-08	2.19E-06	4.85E-14	2.49E-06	1.90E-11	3.05E-09	2.35E-06	1.66E-09	-5.629	1.42E 03
6.75E-11	5.04E-09	1.55E-06	3.43E-14	1.76E-06	6.73E-12	2.16E-09	1.66E-06	1.15E-09	-5.780	1.45E 03
3.37E-11	2.52E-09	1.09E-06	2.42E-14	1.25E-06	2.38E-12	1.52E-09	1.17E-06	7.96E-10	-5.931	1.47E 03
1.69E-11	1.26E-09	7.74E-07	1.71E-14	8.82E-07	8.41E-13	1.08E-09	8.29E-07	5.56E-10	-6.081	1.49E 03
8.44E-12	6.29E-10	5.47E-07	1.21E-14	6.23E-07	2.97E-13	7.62E-10	5.86E-07	3.90E-10	-6.232	1.50E 03
4.22E-12	3.15E-10	3.87E-07	8.57E-15	4.41E-07	1.05E-13	5.39E-10	4.14E-07	2.74E-10	-6.383	1.51E 03
2.11E-12	1.57E-10	2.74E-07	6.06E-15	3.12E-07	3.72E-14	3.81E-10	2.93E-07	1.93E-10	-6.533	1.52E 03
1.05E-12	7.87E-11	1.93E-07	4.28E-15	2.20E-07	1.31E-14	2.69E-10	2.07E-07	1.36E-10	-6.684	1.52E 03
5.27E-13	3.93E-11	1.37E-07	3.03E-15	1.56E-07	4.65E-15	1.91E-10	1.46E-07	9.58E-11	-6.835	1.53E 03
2.64E-13	1.97E-11	9.67E-08	2.14E-15	1.10E-07	1.64E-15	1.35E-10	1.03E-07	6.76E-11	-6.985	1.53E 03
1.32E-13	9.83E-12	6.84E-08	1.51E-15	7.79E-08	5.81E-16	9.53E-11	7.32E-08	4.78E-11	-7.136	1.53E 03
6.59E-14	4.92E-12	4.84E-08	1.07E-15	5.51E-08	2.05E-16	6.74E-11	5.17E-08	3.37E-11	-7.286	1.53E 03
3.30E-14	2.46E-12	3.42E-08	7.57E-16	3.90E-08	7.26E-17	4.76E-11	3.66E-08	2.39E-11	-7.437	1.53E 03
1.65E-14	1.23E-12	2.42E-08	5.35E-16	2.76E-08	2.57E-17	3.37E-11	2.59E-08	1.69E-11	-7.587	1.53E 03
8.24E-15	6.15E-13	1.71E-08	3.79E-16	1.95E-08	9.07E-18	2.38E-11	1.83E-08	1.19E-11	-7.738	1.53E 03
4.12E-15	3.07E-13	1.21E-08	2.68E-16	1.38E-08	3.21E-18	1.68E-11	1.29E-08	8.42E-12	-7.888	1.54E 03
2.06E-15	1.54E-13	8.55E-09	1.89E-16	9.74E-09	1.13E-18	1.19E-11	9.15E-09	5.96E-12	-8.039	1.54E 03
1.03E-15	7.68E-14	6.05E-09	1.34E-16	6.89E-09	4.01E-19	8.42E-12	6.47E-09	4.21E-12	-8.189	1.54E 03
5.15E-16	3.84E-14	4.28E-09	9.47E-17	4.87E-09	1.42E-19	5.95E-12	4.57E-09	2.98E-12	-8.340	1.54E 03
2.57E-16	1.92E-14	3.02E-09	6.69E-17	3.44E-09	5.01E-20	4.21E-12	3.23E-09	2.11E-12	-8.490	1.54E 03
1.29E-16	9.60E-15	2.14E-09	4.73E-17	2.44E-09	1.77E-20	2.98E-12	2.29E-09	1.49E-12	-8.641	1.54E 03
6.44E-17	4.80E-15	1.51E-09	3.35E-17	1.72E-09	6.26E-21	2.11E-12	1.62E-09	1.05E-12	-8.791	1.54E 03
3.22E-17	2.40E-15	1.07E-09	2.37E-17	1.22E-09	2.21E-21	1.49E-12	1.14E-09	7.44E-13	-8.942	1.54E 03

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