The Solubility of Oxygen and Ozone in Liquids

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This review covers the solubility of oxygen and ozone in liquids as a function of temperature and pressure. Solubility data for individual systems were critically evaluated and recommended or tentative values presented in many cases. The trend of solubilities in homologous series or related solvents is discussed. Liquids include water; seawater; aqueous salt solutions; mixed solvents; hydrocarbons; organic compounds containing oxygen, halogen, sulfur, nitrogen, or silicon; olive oil; and human blood. For ozone, only its solubility in water is presented.

Key words: aqueous solutions; biological fluids; gas solubility; hydrocarbons; mixed solvents; organic solvents; oxygen; ozone; seawater; water.

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1. Introduction

This review covers the solubility of oxygen and ozone in most liquids and solutions for which data are available and at all temperatures and pressures. The fluids considered include pure liquids, liquid mixtures, aqueous and organic solutions, and biological fluids. The fluids not considered include molten salts, alloys, metals, glasses, and slags as well as polymeric materials. The literature beginning with Henry in 1803 has been systematically searched, and our coverage includes articles published through the end of 1980. However, since this is a critical review we will not cite all of the papers published for a given gas/liquid system, but just those which present data that are precise enough to contribute to the recommended or tentative values. For the most recent comprehensive coverage of the literature see Ref. 1. We would appreciate hearing about omissions.

Other compilations or reviews relevant to this one are those of Markham and Kobe[2] (general through 1940), Battino and Clever[3] (general through 1966), Clever and Battino[4] (general through 1974), Wilhelm and Battino[5] (thermodynamic functions at 25 °C), and Wilhelm, Battino, and Wilcock[6] (low-pressure for 57 gases in water), the two books by Gerrard[7,8] (comprehensive annotated surveys emphasizing the "R-line"), Kertes *et al.*[9] (general review), Stephen and Stephen[10] (data tables), Seidell[11] (data tables), Landolt/Börnstein Tabellen[12] (data tables), the International Critical Tables,[13] and the IUPAC volume on oxygen and ozone solubilities.[1] In addition, the books by Prausnitz[14] and by Hildebrand, Prausnitz, and Scott[15] have excellent chapters on gas solubilities.

No data for the solubility of oxygen in heavy water were found[105]—this system should be studied. There is also a paucity of high pressure data, no doubt for the simple reason that under these conditions the dissolution vessel may become a bomb calorimeter or reaction vessel due to the high reactivity of compounds with oxygen.

2. Methods of Measurement

Most gas solubility measurements are done by physical means using manometers, burets, and calibrated volumes. Gas chromatography has also been used. The physical methods range in precision from a few per cent to the high-precision apparatus developed by Benson and Krause[17] which is capable of hundredths of a per cent precision. We would classify precisions of 1%–2% as being routine, 0.1%–0.2% as being excellent and less than 0.1% as outstanding. (Only Benson and co-workers and Battino and co-workers have achieved the last standard). Although gas chromatography has been used for many gas solubility measurements, the precision is generally poor, rarely exceeding 3%. Readers interested in the methods used for determining gas solubilities in the individual papers cited in this article should refer either to the original paper or to Ref. 1 which briefly describes methods of measurement for each paper.

Oxygen and ozone solubilities may also be determined by chemical means. Modifications of the Winkler method are the most commonly used for oxygen, particularly in water and seawater. The modified Winkler method is capable of precisions better than 1% if carried out carefully. Also, there are commercially available many devices that utilize the principle of the Clark (polarographic) electrode to determine oxygen concentrations in solution directly by electrochemical means. The precision of this approach is about one per cent. The special problems connected with determining ozone solubilities in water are discussed in Sec. 5.1.

3. Treatment of the Solubility Data

The reviews[1–4,9] discuss solubility units and how they are derived and interrelated. Gerrard[7,8] has a special approach to gas solubility and units and bases his analyses on the "R-line," a reference line modeled after Raoult's law.

3.1. Solubility Units

Gas solubilities have been presented in many different formats, some peculiar to specialized research areas. The physical quantities we have chosen for presenting data are the mole fraction at 101.325 kPa partial pressure of gas (or other pressure where specified) and the Ostwald coefficient L. The latter is defined by Eq. (1) where V_g is the volume of gas absorbed by the volume of absorbing liquid (not solution) V_1, both measured at the same temperature.

$$L = V_g/V_1. \tag{1}$$

If the gas behaves ideally (within the limits or error of the measurement) and if Henry's law is applicable, then the Ostwald coefficient is independent of the partial pressure of the gas. However, it is useful to specify the pressure conditions of the experiment. (Note that some authors define the Ostwald coefficient as the ratio of the concentration of the gas in the liquid phase divided by the concentration in the gas phase. Also see Ref. 106.) The mole fraction of a gas in the solution is related to the Ostwald coefficient by the following equation:

$$x_1 = \left[\frac{1}{V_1^\circ L}\left(\frac{RT}{P_g} + B_{11}\right) + 1\right]^{-1}, \tag{2}$$

where V_1° is the molar volume of the pure liquid, R is the gas constant, T the temperature, P_g the partial pressure of the gas, B_{11} the second virial coefficient of the gas. B_{11} for oxygen[16] varies smoothly from $-45\ \mathrm{cm^3\ mol^{-1}}$ at 200 K to $-1.0\ \mathrm{cm^3\ mol^{-1}}$ at 400 K. This converts to correction factors of 0.27% at 200 K, 0.063% at 300 K, and 0.003% at 400 K (assuming 101.325 kPa). Aside from the oxygen solubilities determined with exceptional precision by B. B. Benson and co-workers (who made real gas correlations in their work), the B_{11} term is negligible.

The Bunsen coefficient α which is defined as the gas volume at STP (101.325 kPa and 273.15 K) absorbed per volume of pure liquid at the temperature of the measurement is related to the Ostwald coefficient by

$$\alpha = 273.15\,L/T. \tag{3}$$

The general formulation of Henry's law is

$$p_1 = K_H x_1, \tag{4}$$

where K_H is the Henry's law constant and p_1 is the partial pressure of the gas. Strictly speaking, Henry's law is a limiting law (for $p \to 0$) although in its simple form in Eq. (4) it has been shown to be applicable in limited pressure ranges in many cases. (See Gerrard[7,8] for counter arguments and examples.) In this paper the relevant form of Henry's law will be explicity identified where it is used.

Finally, any specialty units not described above will be discussed where cited. Where feasible we converted the quantities used in the original paper to mole fractions and Ostwald coefficients and the units to SI.

3.2. Reliability Estimates

The precision of the data has been estimated by us based on the authors' statements, comparison with other workers, and our own judgment. Precision is reported in terms of one standard deviation unless otherwise specified.

3.3. Fitting Equations

All fitting has been done by least squares analysis to the following form where $\tau = T/100$ K:

$$\ln x_1 = A_0 + A_1/\tau + A_2 \ln \tau + A_3\tau + A_4\tau^2. \tag{5}$$

The terms in this equation have been derived from the work of Valentiner, van't Hoff, Clarke and Glew, and R. F. Weiss. Benson and Krause[17] prefer a smoothing equation which fits $-\ln x_1$ to a power series in $1/(T/\mathrm{K})$. Although this power series sometimes fits data with fewer coefficients than Eq. (5), we prefer Eq. (5) since we consider the thermodynamic functions derived from it to be better behaved than those derived from the power series form. For example, the two-term fit in $1/(T/\mathrm{K})$ implies a zeroth-order temperature dependence for the heat capacity.

3.4. Thermodynamic Functions

The thermodynamic functions that are obtained by taking appropriate derivatives of Eq. (5) may be calculated from

$$\Delta\overline{G}_1^\circ = -A_0R\,(T/\mathrm{K}) - 100A_1R - A_2R\,(T/\mathrm{K})\ln(T/100\ \mathrm{K}) - A_3R\,(T/\mathrm{K})^2/100, \tag{6}$$

$$\Delta\overline{S}_1^\circ = A_0R + A_2R\,\ln(T/100\ \mathrm{K}) + A_2R + 2A_3R\,(T/100\ \mathrm{K}), \tag{7}$$

$$\Delta\overline{H}_1^\circ = -100A_1R + A_2R\,(T/\mathrm{K}) + A_3R\,(T/\mathrm{K})^2/100, \tag{8}$$

$$\Delta\overline{C}_{p_1}^\circ = A_2R + 2A_3R\,(T/100\ \mathrm{K}). \tag{9}$$

These thermodynamic functions refer to the change in the property upon transfer of gas from the vapor phase at 101.325 kPa partial pressure to the (hypothetical) solution phase of unit mole fraction. For most of the systems reported herein only two constants are needed to fit the data, three constants are required infrequently, and four constants are needed only in cases of unusual precision and/or curvature.

4. Oxygen Solubility Data up to 200 kPa

In this section we present solubility data up to about 200 kPa partial pressure of gas in subsections by solvent. The order of presentation can be seen in the table of contents. The presented data are smoothed and presented by groups as well as for individual solvents or solutions.

4.1. Oxygen in Water

The solubility of oxygen in water has been the subject of many papers since the early measurements by Bunsen. The bulk of the work concerns oxygen at pressures near atmospheric and temperatures below 348 K. This presentation of recommended solubility values is, therefore, divided into two temperature ranges: below 348 K (Table 1) and above 348 K (Table 3).

Table 1 is a summary of recommended solubility values determined from a critical survey of over 40 papers. From these, 25 papers were excluded as containing data more than two standard deviations from a smooth curve. The 149 selected data points in the remaining 15 papers were then smoothed by Eq. (5).

In addition to values for the mole fraction, the Ostwald coefficients and C values are shown in Table 1. The solubility term C is defined by the equation

$$C/\mathrm{mL(STP)L}^{-1} = \frac{(x_1)(4.689\times 10^6)}{V_T^\circ/\mathrm{mL^3mol}^{-1}}, \qquad (10)$$

where the mole fraction x_1 is at 101.325 kPa partial pressure of oxygen, V_T° is the molar volume of pure water at temperature T, and the ratio of oxygen in air is assumed to be 20.94%. Thus C is the number of milliliters of gas at STP from air dissolved in one liter of solvent. Table 1 also includes as a convenience the values for the molar volume of pure water at selected temperatures. These values are often used to calculate solubility in units other than those already tabulated, and were obtained from Kell's equation for the density of pure water.[18] For temperatures below 348 K, the fitting equations are

$$\ln x_1 = -64.21517 + 83.91236/\tau + 23.24323 \ln(\tau), \qquad (11)$$

$$\ln L = -58.51653 + 84.5991/\tau + 24.41285 \ln(\tau), \qquad (12)$$

$$\ln C = -52.16764 + 84.59929/\tau + 23.41230 \ln(\tau). \qquad (13)$$

The 15 sources for the solubility data used in Table 1 are Refs. 17, and 19–32. The data used from each are shown below by (reference number—number of data points used): (17—21), (19—37), (20—26), (21—14), (22—2), (23—15), (24—1), (25—3), (26—14), (27—1), (28—1), (29—1), (30—8), (31—3), (32—2).

Table 1. Solubility of oxygen in water for the temperature range of 273.15 - 348.15 K and partial pressure of gas of 101.325 kPa[a]

T /K	V_2°/mL mol^{-1}	10^5x_1[b]	10^2L[b]	C[b]/mL(STP)L^{-1}	10^5x_1[c]
273.15	18.018	3.949	4.913	10.277	3.958
278.15	18.016	3.460	4.384	9.005	3.465
283.15	18.020	3.070	3.958	7.988	3.075
288.15	18.031	2.756	3.614	7.167	2.761
293.15	18.047	2.501	3.333	6.498	2.508
298.15	18.068	2.293	3.104	5.951	2.301
303.15	18.094	2.122	2.918	5.499	2.131
308.15	18.123	1.982	2.766	5.128	1.991
313.15	18.156	1.867	2.643	4.822	1.874
318.15	18.193	1.773	2.545	4.570	1.778
323.15	18.233	1.697	2.468	4.364	1.697
328.15	18.276	1.635	2.409	4.195	1.631
333.15	18.323	1.586	2.367	4.059	1.575
338.15	18.372	1.549	2.339	3.953	1.530
343.15	18.425	1.521	2.325	3.871	1.493
348.15	18.480	1.502	2.322	3.811	1.463

[a] See text for comments.

[b] Smoothed values from fifteen sources using eqs (11), (12), and (13), respectively.

[c] Smoothed values using eq (15) from reference [19].

Table 2. Thermodynamic functions for dissolving oxygen at 101.325 kPa pressure in water in the temperature range 273.15 - 348.15 K[a]

T/K	$\Delta\bar{G}_1^\circ$/kJ mol^{-1}	$\Delta\bar{H}_1^\circ$/kJ mol^{-1}	$\Delta\bar{S}_1^\circ$/ J mol^{-1}K^{-1}
273.15	23.02	-17.20	-147.3
278.15	23.75	-16.18	-143.6
283.15	24.46	-15.16	-139.9
288.15	25.15	-14.15	-136.4
293.15	25.83	-13.13	-132.9
298.15	26.48	-12.11	-129.5
303.15	27.12	-11.10	-126.1
308.15	27.74	-10.08	-122.7
313.15	28.35	-9.06	-119.5
318.15	28.94	-8.05	-116.3
323.15	29.51	-7.03	-113.1
328.15	30.07	-6.01	-110.0
333.15	30.61	-5.00	-106.9
338.15	31.14	-3.98	-103.9
343.15	31.65	-2.97	-100.9
348.15	32.15	-1.95	-97.9

[a] See text for comments; using coefficients in eq (11).

Fitting all 149 points by Eq. (5) gave a standard deviation of ± 0.36%. Considering the variety of both chemical and physical techniques used to measure the solubility, and the number of data points, this fit shows an amazing consistency. The recommended values in Table 1 are believed to be accurate to about ± 0.3%. (See next section.)

From the coefficients A_0, A_1, and A_2 in Eq. (11), the thermodynamic functions can be calculated according to Eqs. (6)–(9). Note that for a three term fit, the value for $\Delta\bar{C}_p^\circ$ is constant at 203 J mol^{-1} K^{-1} over this temperature range within the precision of the data. The Gibbs energy, enthalpy, and entropy changes are listed in Table 2.

The solubility of oxygen in water at temperatures above 348 K were investigated by Stephan *et al.*[33] and Pray *et al.*[34] Their data were fitted by Clever and Han,[35] together with lower temperature data to yield:

$$\ln x_1 = -54.0411 + 68.8961/\tau + 18.554 \ln(\tau). \qquad (14)$$

Table 3. Solubility of oxygen in water for the temperature range 348.15 - 573.15 K and partial pressure of 101.325 kPa[a]

T/K	10^5 x_1	T/K	10^5 x_1
348.15	1.502	433.15	1.780
353.15	1.478	453.15	2.038
358.15	1.462	473.15	2.388
363.15	1.450	493.15	2.852
368.15	1.445	513.15	3.460
373.15	1.444	533.15	4.250
393.15	1.487	553.15	5.276
413.15	1.599	573.15	6.603

[a] See text for comments.

Values for the mole fraction of dissolved oxygen at selected temperatures are shown in Table 3. The precision of these values is poorer than those below 348 K, and is estimated to be ± 2.0%.

4.1.a. Oxygen/Water as a Recommended Reference System

We recommend the system of oxygen dissolved in water as a reference system since it is the most commonly measured and most precisely known gas solubility. While the data in Table 1 summarize the best available solubility values derived from many sources and thus are appropriate for general use, recent work shows much better precision than the 0.3% associated with Table 1. Therefore, new methods with high precision should use the smoothed values from Benson *et al.*[19] for comparison. They proposed the following fitting equation between 273 and 373 K:

$$-\ln x_1 = 3.71814 + 5.59617\times 10^3/(T/\mathrm{K}) - 1.049668\times 10^6/(T/\mathrm{K})^2 \qquad (15)$$

or when the data are refitted by Eq. (5):

$$\ln x_1 = -64.21517 + 83.91236/\tau + 23.24323 \ln(\tau). \qquad (16)$$

The standard deviation from the fitting equation is ± 0.017%, which is by far the most precise measurement of gas solubility to date.

Benson *et al.*[19] determined a mole fraction x_1 of 2.301×10^{-5} at 298.15 K and 101.325 kPa partial pressure of oxygen. This value is 0.35% higher than that given in Table 1, but the historical trend has been towards higher mole fraction values.[3,6] Since this is the most precise and probably most accurate gas solubility measurement available, all future tests of methods should include values for the system of oxygen in water for comparison. Smoothed values from Eq. (15) are given in Table 1.

Mortimer[36] recently presented a critical review of oxygen solubilities in fresh waters with many tables, nomographs, etc. His recommendations are based on the work of Benson *et al.*[19]

4.2. Oxygen in Seawater

The solubility of oxygen in seawater has been studied nearly as widely as the solubility in pure water, but with less agreement among the data provided by different researchers. The most reliable data appear to be those from Carpenter[20] and Murray and Riley,[26] with measurements between 0 and 36 °C and 0% to 40% salinity.

Table 4. Coefficients for eq (19) for several solubility units for oxygen in seawater

Coefficients	mL(STP)/L	mL(STP)/kg	mol/kg
A_1	-1268.9782	-1286.2408	-1282.8704
A_2	36063.19	36607.82	36619.96
A_3	220.1832	223.0650	223.1396
A_4	-0.351299	-0.354587	-0.354707
B_1	6.229×10^{-3}	5.954×10^{-3}	5.957×10^{-3}
B_2	-3.5912	-3.7341	-3.7353
B_3	3.44×10^{-6}	3.68×10^{-6}	3.68×10^{-6}

Table 5. Values of C in mL oxygen (STP) per liter seawater for selected temperatures and salinities.

T/K	Salinity/%								
	0	5	10	15	20	25	30	35	40
273.15	10.216	7.2908	5.2936	3.9102	2.9384	2.2464	1.7472	1.3825	1.1129
278.15	8.9185	6.4406	4.7319	3.5368	2.6894	2.0805	1.6374	1.3110	1.0679
283.15	7.8852	5.7597	4.2801	3.2358	2.4887	1.9474	1.5502	1.2554	1.0343
288.15	7.0472	5.2045	3.9104	2.9890	2.3243	1.8388	1.4800	1.2118	1.0095
293.15	6.3557	4.7440	3.6024	2.7830	2.1873	1.7489	1.4227	1.1774	0.9912
298.15	5.7754	4.3554	3.3415	2.6081	2.0709	1.6730	1.3750	1.1496	0.9779
303.15	5.2803	4.0218	3.1164	2.4566	1.9702	1.6075	1.3343	1.1268	0.9680
308.15	4.8511	3.7306	2.9186	2.3230	1.8810	1.5495	1.2986	1.1072	0.9604
313.15	4.4731	3.4720	2.7417	2.2026	1.8002	1.4968	1.2662	1.0896	0.9540

The difficulties with seawater measurements are both in analysis and interpretation. The measurement of oxygen in seawater was often complicated due to the loss of iodine and interferences within the chemical methods of analysis. For this reason, much of the early work was excluded. The multitude of components in seawater also precluded a treatment of the data via Setchenow's equation (which follows) for concentration effects for each ionic species:

$$\log \frac{y_\mathrm{i}}{y_\mathrm{i}^\circ} = \log \frac{S_\mathrm{i}^\circ}{S_\mathrm{i}} = k_\mathrm{s} C_\mathrm{s}. \qquad (17)$$

S_i and S_i° are the solubilities and y_i and y_i° are the activity coefficients of the gas in the salt solution and pure solvent, respectively. C_s is the electrolyte concentration and k_s is the salt effect parameter.

As a simplification, Weiss[37] proposed the following equation:

$$\ln C = A_1 + A_2/\tau + A_3 \ln(\tau) + A_4\tau + S[B_1 + B_2\tau + B_3\tau^2], \qquad (18)$$

where solubility C is given by Eq. (10) and S is salinity in parts per thousand. The A terms in Eq. (18) resemble the normal Weiss Eq. (5), while the additional B terms fit the salinity dependence. In their analysis of oxygen solubility in seawater, Chen and Carpenter[38] showed that Eq. (19) was superior to Eq. (18).

$$\ln C = A_1 + A_2/(T/\mathrm{K}) + A_3 \ln(T/\mathrm{K}) + A_4(T/\mathrm{K}) + S[B_1 + B_2/(T/\mathrm{K})] + B_3 S^2. \qquad (19)$$

The concentration term C can have the different units shown in Table 4, with the corresponding coefficients.

The values generated from Eq. (19) with the coefficients in Table 4 (see Table 5) are valid only between 9 and 35 °C, below 400 ppt salinity and relatively low pressures. Solubility studies with higher salinity (marine brines) by Kinsman *et al.*,[39] are imprecise and unconfirmed and thus are not included in this summary.

4.3. Oxygen in Aqueous Salt Solutions

The "salting-in" or "salting-out" of a nonelectrolyte solute is a common phenomenon. One way of expressing the effect of a dissolved electrolyte on the solubility of oxygen in water is the Setschenow salt parameter k_s. If the concentration of the electrolyte is c_2 (mol L^{-1}) and the gas solubility is expressed as the Bunsen coefficient α^0 in pure water and α in the electrolyte solution, the salt effect parameter is

$$k_{sc\alpha} = (1/c_2) \log(\alpha^0/\alpha). \tag{20}$$

Other units of concentration and gas solubility will result in equivalent salt effect parameters.

The Setschenow equation (20) is an approximation based upon a large solubility difference between the electrolyte and nonelectrolyte solutes. This is a good approximation for oxygen dissolved in water. Plots of $\log(\alpha^0/\alpha)$ versus c_2 are often linear over a modest range of electrolyte concentrations. However, at high concentrations of electrolyte, these plots can become highly curved.

Except for the high pressure studies by Bruhn, Gerlach, and Pawlek,[40] the solubility of oxygen was determined at pressures near 101.325 kPa. Whenever possible, the individual author's value for α^0 is used instead of those suggested earlier in this work in the hope that the ratio (α^0/α) might cancel out any systematic errors.

The electrolytes are discussed in the following groups: acids, bases, Group IA salts, Group IIA salts, and others. Due to the scatter observed in these data, and the frequent lack of any similar studies, the values given in this section should be considered only as tentative.

4.3.a. Acids

The acids considered are hydrochloric, sulfuric, and nitric. The values for the Setschenow salt effect parameter for the first two acids are shown in Table 6 and are from Geffcken.[22] The salt effect parameter appears to decrease with temperature and also with increasing sulfuric acid concentration. Geffcken, who investigated concentrations from 0.2 to 2.6 mol L^{-1}, noted only a slight decrease, but data from Bohr[41] show a more pronounced falloff of $k_{sc\alpha}$ for concentrations ranging up to 18 mol L^{-1}.

The solubility of oxygen in 1.0 mol L^{-1} aqueous sulfuric acid was measured over a wide temperature range by Bruhn, Gerlach, and Pawlek.[40] Values for $k_{sc\alpha}$ remained nearly constant at 0.10 L mol^{-1} for temperatures between 323 and 523 K.

Nitric acid is a case of special interest. Values of $k_{sc\alpha}$ for a 1.0 mol L^{-1} solution are shown in Table 7. The most extensive study was by Pogrebnaya, Usov, and Baranov[42] who measured oxygen solubility from 283 to 333 K for concentrations of nitric acid from 0 to 12 mol L^{-1}. For the lower temperature and concentration regions, nitric acid behaves like hydrochloric and sulfuric acid, salting out oxygen. But at higher concentrations at the same temperature, a salting-in effect is observed. At 323 K, the salting-in phenomenon occurs above 10 mol L^{-1}, and at 333 K, it occurs above 8 mol L^{-1}. At mole fractions of nitric acid below 0.16, the solubility of oxygen decreases with increasing temperature. At higher mole fractions, oxygen becomes more soluble with increasing temperature.

Table 6. Setschenow salt effect parameters for hydrochloric and sulfuric acids

Acid (1.0 mol L^{-1})	$k_{sc\alpha}$ (L mol^{-1}) 288.15 K	298.15 K
HCl	0.044	0.031
H_2SO_4	0.105	0.087

Table 7. Setschenow salt effect parameters for 1.0 mol L^{-1} nitric acid at 283.15 - 333.15 K

T/K	k_{sc} (L mol^{-1})
283.15	0.0440
293.15	0.0255
303.15	0.0175
313.15	0.0115
323.15	0.0090
333.15	0.0050

4.3.b. Bases

Strong bases such as Group IA hydroxides have a pronounced effect on the solubility of oxygen. Khomutov and Konnik[43] examined all the alkali metal hydroxides and their results are summarized in Table 8. The two results for lithium hydroxide reflect two different linear salting-out regions, the lower concentration one being proportionately more effective. Recent work by Broden and Simonson[44] show a similar pattern for sodium hydroxide. A plot of $\log(\alpha^0/\alpha)$ versus c_2 between 0.01 and 0.10 mol L^{-1} is linear but with an anomalously high slope of 0.65 L mol^{-1}. At higher concentrations of sodium hydroxide, Geffcken[22] and Bruhn, Gerlach, and Pawlek,[40] calculate slopes near 0.180 in agreement with Khomutov and Konnik.[43] The values of $k_{sc\alpha}$ computed by Yasunishi[45] are somewhat lower.

Khomutov and Konnik's value for potassium hydroxide is supported by the results of Geffcken,[22] Shoor *et al.*[46] and Knaster and Apel'baum,[47] with no evidence yet found for more than one slope. The value of $k_{sc\alpha}$ proposed by MacArthur[48] is lower than all the others and can be rejected. Khomutov and Konnik's[43] paper is the only published research for rubidium and cesium hydroxide salt effects.

As expected, a weak base such as ammonium hydroxide has a very small salt effect parameter, nearly constant at 0.006 L mol^{-1} despite varying concentration from 0 to 8 mol L^{-1}.[40]

Table 8. Setschenow salt effect parameters for various alkali metal hydroxides at 298.15 K

Salt	Concentration (mol L^{-1})	$k_{sc\alpha}$ (L mol^{-1})
LiOH	0 - 0.07	0.332
LiOH	0.12 - 1.2	0.091
NaOH	1.2	0.181
KOH	0.8	0.176
RbOH	0.5	0.168
CsOH	0.5	0.158

4.3.c. Group IA Cations

With the single exception of high concentrations of lithium fluoride, all alkali metal halides act to salt-out dissolved oxygen. As previously noted with lithium hydroxide, two distinct regions of linear salt effects exist for lithium halides except lithium iodide. The values for $k_{sc\alpha}$ and the related concentration ranges are shown in Table 9. Results from several investigations are shown for sodium and potassium chloride. The general trend for the alkali metal halides is toward a smaller salt effect parameter when increasing the size of either the cation or anion.

Other common salts of the alkali metals are listed in Table 10. Lithium nitrate salts-in oxygen at higher concentrations, and along with lithium perchlorate shows two linear regions of salt effects. The multiply charged sulfate, phosphate, and carbonate anions have a higher ionic strength and show larger salt effect parameters than do perchlorate and nitrate. A report of oxygen solubility in sodium acetate solution of varying pH was made by Guseva *et al.*,[50] but without sufficient information to calculate $k_{sc\alpha}$. The higher temperature and pressure study by Broden and Simonson[44] shows two regions for sodium bicarbonate salt effect. At 323 K and pressures about 1 MPa, $k_{sc\alpha}$ was equal to 0.3 L mol^{-1} for concentrations up to 0.1 mol L^{-1}, but $k_{sc\alpha}$ was equal to 0.14 L mol^{-1} at higher concentrations. The Broden and Simonson[44] values should be considered tentative.

Mixtures of electrolytes including Group IA cations have been studied to a very limited extent. Murray, Riley, and Wilson[25] observed a salting-out effect for a mixture of sodium iodide and sodium hydroxide equivalent to 0.180 L mol^{-1} of total electrolyte concentration, which is the tenative value for sodium hydroxide itself. A similar result was observed for sodium sulfate and sulfuric acid by Kobe and Kenton[51] and for sodium sulfate, sodium dithionite, and sodium hydroxide in solution by Jhaveri and Sharma.[52]

Table 9. Values of k_{sc} for alkali metal halides at 298.15 K[a,b]

	F	Cl	Br	I
Li	0.725 (0–.01)[c] -0.385 (0.04–.10)[c]	0.112 (0–.07)[c] 0.070 (.15–1.2)[c]	0.252 (0–.07)[c] 0.084 (.15–1.2)[c]	0.163
Na	0.284	0.145 0.141[22] 0.138[48]	0.131	0.120
K	0.203	0.129 0.128[48] 0.094[49]	0.117	0.093
Rb	0.146	0.120	0.104	0.086
Cs	0.114	0.098	0.078	0.062

[a] values from [43] unless otherwise noted. These values should be considered tentative. One puzzling point is that Khomutov and Konnick [43] report data for a LiF concentration of 0.10 M whereas the *solubility* is about 0.03 M.
[b] units of $k_{sc\alpha}$ are L mol^{-1}.
[c] concentration range in mol L^{-1} where $k_{sc\alpha}$ observed.

Table 10. Values of $k_{sc\alpha}$ for alkali metal salts at 298.15 K[a,b]

	ClO_4^-	$SO_4^=$	NO_3^-	PO_4^{-3}	$CO_3^=$
Li	0.218 (0–.07)[c] 0.066 (.15–1.2)[c]	0.244	0.196 (0–.07)[c] -0.040 (.15–1.2)[c]		0.254
Na	0.160	0.376 0.398[45] 0.325[48]	0.124	0.652	0.356 0.338[45] 0.464[44]
K	0.150	0.297 0.345[22] 0.345[48]	0.105	0.507	0.379
Rb	0.150	0.290	0.096		
Cs		0.225	0.066		

[a] values from [43] unless otherwise noted.
[b] units of $k_{sc\alpha}$ are L mol^{-1}.
[c] concentration range in mol L^{-1} where $k_{sc\alpha}$ observed.

4.3.d. Group IIA Cations

Five salts of alkaline earth metals have been examined for their effect on the solubility of dissolved oxygen. They are magesium chloride, calcium chloride, barium chloride, magnesium sulfate, and calcium nitrate. At 298.15 K and concentrations below about 2 mol L^{-1}, Yasunishi[45] found the $k_{sc\alpha}$ values to be 0.200, 0.273, 0.204, 0.194, and 0.270 L mol^{-1}, respectively. When results from concentrations ranging from 2 to 4 mol L^{-1} were included in the data base, a better fit was achieved for magnesium chloride, magnesium sulfate, and calcium chloride using the equation:

$$\frac{k^0_{sc\alpha}}{1+k'_{sc\alpha}c_2}=\left(\frac{1}{c_2}\right)\log\left(\frac{\alpha^0}{\alpha}\right). \tag{21}$$

Specific values are given in Table 11.

Table 11. Values for salt effect parameters in eq (21) for Group IIA metal salts[a]

	$MgCl_2$	$MgSO_4$	$CaCl_2$
$k^o_{sc\alpha}$	0.222	0.250	0.226
$k'_{sc\alpha}$	0.0566	-0.0583	0.0523

[a] The $MgCl_2$ data are from [53] and the $MgSO_4$ and $CaCl_2$ are from [45].

4.3.e. Other Cations

Bruhn, Gerlach, and Pawlek[40] reported salt effect parameters for various salts at elevated temperature and pressure. The results are summarized in Table 12. All the electrolytes salt-out oxygen, with little effect of temperature.

Morrison and Johnstone[54] have shown that tetraethyl ammonium bromide has a mild salting-in effect, with $k_{sc\alpha}$ equal to -0.04 L mol^{-1}. As expected, the highly charged electrolyte $Al_2(SO_4)_3$ has a large salt effect parameter equal to 0.745 L mol^{-1}.[45] The same study reports that concentrations of aluminum chloride up to 1.7 mol L^{-1} can be fitted by Eq. (20) to yield $k_{sc\alpha}$ of 0.274 L mol^{-1}. But including concentrations up to 2.2 mol L^{-1}, Eq. (21) provides a better fit with $k^0_{sc\alpha} = 0.303$ and $k'_{sc\alpha} = 0.0859$. Murray, Riley, and Wilson[25] have shown that manganese chloride and manganese sulfate have salt effect parameters of 0.202 and 0.194 L mol^{-1}, respectively.

Colloidal solutions of hydrated iron oxide,[55] uranyl fluoride,[33] and uranyl sulfate[30,33] solutions have been used in oxygen solubility tests, but the salt effect parameters were not obtained. Mixed solutions of uranyl sulfate, sulfuric acid, and copper sulfate[56] showed no obvious salting-out effects, but this may be due to the low concentrations used in the study.

Table 12. Values of $k_{sc\alpha}$ for selected sulfate salts at 298–423 K

T/K	$(NH_4)_2SO_4$	$CuSO_4$	$NiSO_4$	$CoSO_4$
298	0.212	0.114	0.113	0.115
323	0.196	0.123	0.116	0.128
373	0.203	0.106	0.112	0.105
423	0.193	0.119	0.122	0.117

4.4. Oxygen in Organic Solvents Plus Water

The solubility of oxygen in mixtures of water with polar organic solvents (usually alcohols) has been determined by a number of investigators. Tokunaga[57] has determined oxygen solubilities in methanol/water, ethanol/water, 1-propanol/water, and 2-propanol/water mixtures over the whole composition range and at 273.15, 293.15, and 313.15 K. Cargill[58] determined oxygen solubilities in ethanol/water and t-butanol/water mixtures over the whole composition range and in the temperature range of 277.3 to 334.4 K. Cargill paid particular attention to solubilities at low concentrations of alcohols. We consider Cargill's data to be the most reliable for the ethanol/water mixtures and present our calculated values of the solubilities in terms of the mole fraction at 101.325 kPa partial pressure of oxygen in Table 13. The extensive data reported by Tokunaga may be found in Refs. 1 or 57.

Table 13. Mole fraction solubilities of oxygen in ethanol/water mixtures at 101.325 kPa partial pressure of oxygen

	$10^4\ x_1$									
	T/K									
x_{EtOH}	273.15	277.15	283.15	285.15	293.15	298.15	303.15	313.15	323.15	333.15
0	0.3806	0.3475	0.3046	0.2920	0.2492	0.2280	0.2106	0.1850	0.1690	0.1584
0.008	0.3949	0.3582	0.3115	0.2980	0.2528	0.2312	0.2139	0.1891	0.1738	0.1624
0.021	0.4017	0.3692	0.3265	0.3137	0.2696	0.2472	0.2285	0.2005	0.1833	0.1740
0.032	0.4173	0.3812	0.3354	0.3216	0.2763	0.2542	0.2362	0.2099	0.1931	0.1806
0.063	0.4130	0.3811	0.3399	0.3277	0.2868	0.2668	0.2508	0.2290	0.2186	0.2165
0.097	0.3872	0.3637	0.3337	0.3250	0.2964	0.2828	0.2721	0.2574	0.2492	0.2441
0.120	0.3725	0.3551	0.3337	0.3275	0.3071	0.2976	0.2906	0.2822	0.2799	0.2815
0.162	0.3727	0.3680	0.3615	0.3596	0.3529	0.3501	0.3485	0.3496	0.3576	0.3740
0.229	0.4712	0.4940	0.5064	0.5084	0.5035	0.4971	0.4910	0.5039	0.5236	0.5376
0.31	0.8129	0.8049	0.8016	0.8023	0.8123	0.8219	0.8321	0.8472	0.8450	0.8116
0.493	1.567	1.560	1.556	1.556	1.567	1.581	1.597	1.637	1.679	1.715
0.780	3.421	3.450	3.484	3.492	3.521	3.533	3.544	3.558	3.574	3.599
0.992	5.414	5.475	5.538	5.555	5.593	5.604	5.606	5.600	5.598	5.630

4.5. Oxygen in Hydrocarbons

4.5.a. Saturated Hydrocarbons

Smoothed values of mole fraction solubility for n-pentane, n-hexane, n-heptane, n-octane, n-nonane, n-decane, and 2,2,4-trimethylpentane are given in Table 14. Also shown are the coefficients A_0 and A_1 of Eq. (5), the standard deviation σ, and the number of data points used. In the case of the normal hydrocarbons, the mole fraction solubilities are a very weak function of the temperature ($\Delta\bar{H}_1^\circ \simeq 0$). Although the coefficient A_1 of Eq. (5) is large for n-hexane, n-heptane, and n-nonane, these are considered to be artificial because of the narrow temperature range studied and the experimental uncertainty. The dependence of the mole fraction solubility on the solvent chain length is not clear. From n-undecane to n-octadecane, the Makranczy *et al.* values[59] decrease as a function of hydrocarbon chain length, while the Blanc and Batiste values[60] show the opposite trend. This is demonstrated in Fig. 1. In fact, a least square analysis of 26

Table 14. Mole fraction solubility of oxygen in saturated hydrocarbons at 101.325 kPa partial pressure (10^4x_1)

T/K	n-Hexane	n-Heptane	n-Octane	2,2,4-Trimethyl-pentane	n-Nonane	n-Decane
243.15				30.24		
253.15				29.41		
263.15				28.66		
273.15				27.98		
283.15			21.28	27.37		21.91
293.15	19.6	19.98	21.22	26.81		21.82
298.15	20.5	20.55	21.20	26.54	21.10	21.78
303.15		21.12	21.17	26.29	20.52	21.74
313.15		22.24	21.12	25.82		21.67
323.15				25.38		
A_0^a	-3.524	-4.535	-6.230	-6.508	-7.852	-6.237
A_1^a	-7.948	-4.928	0.219	1.720	5.041	0.322
$10^4\sigma^b$	1.3	0.72	0.45	1.42	0.16	0.28
#^{c}	4	7	7	10	3	4
n-Pentane at 298.15 K: $10^4x_1 = 20.5$ [59]						

[a] Coefficients in eq (5).

[b] Standard deviation.

[c] Numbers of data points used.

[d] See text for references for each solvent.

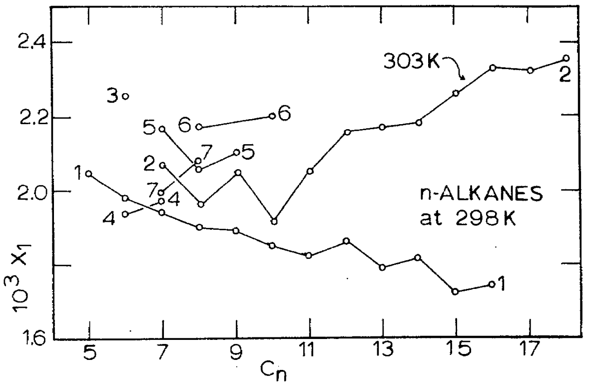

FIGURE 1. Solubility of oxygen in the n-alkanes. The numbers in the figure refer to data taken from the following references: 1 (Ref. 59); 2 (Ref. 60); 3 (Ref. 61); 4 (Ref. 62); 5 (Ref. 63); 6 (Ref. 64); and 7 (Ref. 65).

pairs of data for all of the normal hydrocarbons in Table 14 give $A_0 = -6.020$, $A_1 = -0.442$, and $10^4\sigma = 0.87$.

In the case of 2,2,4-trimethylpentane, the mole fraction solubilities are 20% to 30% higher than those for the normal hydrocarbons. In addition, both the Kobatake and Hildebrand[66] and Kretschmer *et al.*[67] results show a decrease in solubility as the temperature increases ($\Delta \bar{H}_1^\circ < 0$).

Following is a brief description of original data for each solvent.

n-Hexane: smoothed values were obtained by using Naumenko[61] and Makranczy *et al.*[59] values both at 208.15 K, and Guerry's values[62] at 293.15 and 298.15 K.

n-Heptane: The values of Guerry[62] at 293.15 and 298.15 K, Thomsen and Gjaldbaek[63] at 298.15, 298.25, and 307.95 K, Ijams[65] at 298.15 K, and Blanc and Batiste[60] at 303.15 K were used.

n-Octane: Although the values of Wilcock *et al.*[64] are preferred, smoothed values were obtained by using those of Thomsen and Gjaldbaek[63] and Ijams,[65] in addition to those of Wilcock *et al.*

2,2,4-Trimethylpentane: The four values of Kobatake and Hildebrand[66] over the temperature range of 282.87 to 303.36 K give $A_0 = -6.5102$, $A_1 = 1.8995$, and $10^4\sigma = 0.01$. The four values of Kretschmer *et al.*[67] over the temperature range of 248.15 to 323.15 K (which are lower than those of Kobatake and Hildebrand by 8.7%) give $A_0 = -6.6138$, $A_1 = 1.9369$, and $10^4\sigma = 0.53$. The smoothed values were obtained by using the data from both of these papers along with those of Baldwin and Daniel[68] and Ijams.[65]

n-Nonane: The Thomsen and Gjaldbaek values[63] at 298.05 and 298.15 K and the Blanc and Batiste value[60] at 303.15 K were used.

n-Decane: The values of Wilcock *et al.*[64] at 283.15, 298.11, and 313.48 K give $A_0 = -6.2238$, $A_1 = 0.3043$, and $10^4\sigma = 0.04$. Although these values are preferred, smoothed values were obtained by using them along with the Ijams' value at 298.15 K.[65]

4.5.b. Cyclic Hydrocarbons

Smoothed values of mole fraction solubility for a group of cyclic hydrocarbons are given in Table 15. Mole fraction solubility increases in the order cyclohexene < cyclooctane ~ cyclohexane < methylcyclohexane ~ *cis*-1,2-dimethylcyclohexane < trans-1,2-dimethylcyclohexane ~ 1,3-dimethylcyclohexane (*cis* and *trans* mixture) ~ 1,4-dimethylcyclohexane (*cis* and *trans* mixture). Solubilities in these solvents are lower than those in n-alkanes and higher than those in benzene.

The following is a summary of the original data and how they were processed.

Cyclohexane: Wilhelm and Battino[69] report eight points over the temperature range of 283.47 to 313.06 K, which give $A_0 = -6.592$, $A_1 = -0.280$, and $10^4\sigma = 0.10$. Wild *et al.*[70] report 11 points over the temperature range of 312.2 to 371.2 K, which give $A_0 = -6.312$, $A_1 = -1.278$, and $10^4\sigma = 0.12$. Guerry[62] reports two points at 293.15 and

Table 15. Mole fraction solubility of oxygen in cyclic hydrocarbons at 101.325 kPa partial pressure of gas ($10^4 x_1$)

T/K	Cyclohexane[a]	Cyclohexene	Methylcyclohexane	cis-1,2-Dimethylcyclohexane	trans-1,2-Dimethylcyclohexane	1,3-Dimethylcyclohexane[b]	1,4-Dimethylcyclohexane[c]	Cyclooctane
283.15	12.27		15.49					10.98
293.15	12.31	10.4	15.71					10.92
298.15	12.34	10.4	15.82	15.43	17.34	17.22	17.37	10.89
303.15	12.36		15.92	15.40	17.24	17.14	17.32	10.87
313.15	12.39		16.12	15.34	17.05	16.98	17.24	10.81
A_0[d]	-6.599	-6.869	-6.056	-6.596	-6.711	-6.657	-6.512	-6.973
A_1[d]	-0.296	0	-1.172	0.363	1.053	0.873	0.466	0.450
$10^4\sigma$[e]	0.20		0.12					0.12
#[f]	20	2	3	2	2	2	2	3

[a] Temperature range studied: 283-371 K.

[b] Mixture of 59 mol % cis-1,3-Dimethylcyclohexane and 41 mol % trans-1,3-Dimethylcylclohexane.

[c] Mixture if 70 mol % cis-1,4-Dimethylcyclohexane and 30 mol % trans-1,4-Dimethylcyclohexane.

[d] Coefficients in eq (5).

[e] Standard deviation.

[f] Numbers of data points used.

[g] See text for references for each solvent.

298.15 K. All of the data of these three groups except for 1 point of Wild *et al.* at 293.2 K were used to obtain the smoothed values.

Cyclohexene: Only Guerry[62] reports values at 293.15 and 298.15 K.

Methylcyclohexane; *cis*-1,2-Dimethylcyclohexane; *trans*-1,2-Dimethylcyclohexane; mixture of 59 mol % *cis*-1,3-Dimethylcyclohexane and 41 mol % *trans*-1,3-Dimethylcyclohexane; mixture of 70 mol % *cis*-1,4-Dimethylcyclohexane and 30 mol % *trans* 1,4-Dimethylcyclohexane: Only the data of Geller *et al.* are available.[71]

Cyclooctane: Only the data of Wilcock *et al.* are available.[72]

4.5.c. Aromatic Hydrocarbons

The mole fraction solubility increases when an alkyl substituent is introduced on the benzene ring, i.e., from 8.10×10^{-4} for benzene to 15.69×10^{-4} for (1-methylpropyl)benzene, both at 298.15 K. This is shown in Tables 16 and 17. In benzene, the solubility increases as temperature rises, and this corresponds to $\Delta\overline{H}_1^\circ = 1.48$ kJ mol^{-1} at 298.15 K. In methylbenzene and 1,4-dimethylbenzene, the temperature dependence of the solubility is not large compared to experimental uncertainty ($\Delta\overline{H}_1^\circ \simeq 0$).

The following is a summary of how the data were handled.

Benzene: Horiuti[73] reported six values in the temperature range of 283.15 to 333.15 K. Schlapfer *et al.*[74] reported seven values in the temperature range 283 to 343 K. Byrne *et al.*[75] reported four values from 310.6 to 310.7 K. These are in satisfactory agreement and smoothed values were obtained by using six values of Horiuti, seven values of Schlapfer *et al.* and three values of Byrne *et al.* Both the Naumenko value[76] at 298.15 K (which is 8.3% higher than the smoothed value) and the Morgan and Pyne value[77] at 298.15 K (which is 6.4% lower) were omitted.

Table 16. Mole fraction solubility of oxygen in aromatic hydrocarbons at 101.325 kPa partial pressure of gas (10^4x_1)

T/K	Benzene	Methyl-benzene	1,4-Dimethyl-benzene
283.15	7.88		
293.15	8.02	9.17	
298.15	8.10	9.23	11.69
303.15	8.18	9.28	11.67
313.15	8.37	9.38	11.65
323.15	8.57		11.63
333.15	8.80		11.61
343.15	9.05		11.59
353.15			11.57
A_0[a]	-13.9075	-6.639	-6.818
A_1[a]	8.7417	-1.043	0.196
A_2[a]	3.5302		
$10^4\sigma$[b]	0.06	0.20	0.41
#[c]	16	3	7

[a] Coefficients in eq (5).

[b] Standard deviation.

[c] Numbers of data points used.

[d] See text for references for each solvents.

Table 17. Mole fraction solubility of oxygen in aromatic hydrocarbons at 298.15 K and 101.325 kPa partial pressure of gas (10^4x_1)[a]

1,2-Dimethylbenzene	11.18
1,3-Dimethylbenzene	11.96
Ethylbenzene	12.20
Propylbenzene	13.45
(1-methylethyl)benzene	13.88
1-methyl-4-propylbenzene	14.29
Butylbenzene	14.40
(1-methylpropyl)benzene	15.69

[a] [61].

Methylbenzene (Toluene): Only the Field *et al.* data[78] were used to obtain smoothed values. The Naumenko *et al.* value[76] at 298.15 K is 16% higher than the smoothed value of Field *et al.* and was omitted.

1,4-Dimethylbenzene (p-Xylene): Six values of Fisher over the temperature range of 303.2 to 353.2 K[79] and a value of Naumenko *et al.*[76] at 298.15 K were used to obtain the smoothed values.

Other alkylbenzenes: Only Naumenko *et al.* values[76] at 298.15 K are available and they are shown in Table 16.

4.6. Oxygen in Organic Compounds Containing Oxygen

4.6.a. Alcohols

The smoothed values of the mole fraction solubilities are shown in Table 18. For 1-propanol, 1-pentanol, 1-hexanol, 1-nonanol, 1-undecanol, and 1-dodecanol, only the Makranczy *et al.* values are available.[80] However, their values are systematically low when compared with those obtained by other groups and were thus consequently omitted. The solubility increases as function of carbon number (see Fig. 2). The temperature dependence of the solubility is not very large but it decreases as the temperature rises yielding $\Delta\overline{H}_1^\circ$ values of -2.1 kJ mol^{-1} for 2-methyl-1-propanol to -0.5 kJ mol^{-1} for 1-decanol.

The following summarizes how the original data were handled.

Methanol: Only values of Kretschmer *et al.* at 248.15, 273.15, 298.15, and 323.15 K[67] were used to obtain smoothed values. The Makranczy *et al.* value at 298.15 K[80] (which is 8% lower than that of Kretschmer *et al.*) was ignored.

Ethanol: At least eight groups have reported oxygen solubility in ethanol. The original data used to obtain the smoothed values are as follows: four values of Kretschmer *et al.*[67] over the temperature range of 248.15 to 323.15 K were weighted two times; eight values of Schlapfer *et al.*[74] 273 to 343 K; six values of Timofeev,[32] 273 to 290.2 K with the value at 296.55 K omitted; a value of Shchukarev and Tolmacheva[82] at 277.15 K with the omission of three values at higher temperatures; and a value of Naumenko[61] at 298.15

Table 18. Mole fraction solubility of oxygen in alcohols at 101.325 kPa partial pressure (10^4x_1)

T/K	Methanol	Ethanol	2-Propanol	1-Butanol	1-propanol	1-Octanol	1-Decanol
253.15	4.51	6.29					
263.15	4.42	6.17					
273.15	4.33	6.06	8.13	8.33	9.08		
283.15	4.26	5.96	8.00	8.17	8.79	11.6	12.53
293.5	4.19	5.87	7.88	8.03	8.52	11.4	12.43
298.15	4.15	5.83	7.82	7.96	8.40	11.3	12.39
303.15	4.12	5.79	7.77	7.90	8.28		12.35
313.15	4.06	5.70	7.66	7.78	8.05		12.35
323.15	4.01	5.64	7.57	7.67	7.85		12.27
333.15		5.57					
343.15		5.51					
A_0[a]	-8.2471	-7.8738	-7.5774	-7.6234	-7.9459	-7.2361	-6.9018
A_1[a]	1.3742	1.2693	1.2639	1.4554	2.5735	1.3485	0.6215
$10^4\sigma$[b]	0.03	0.11	0.05	0.05	0.08		0.14
#[c]	4	24	3	3	8	2	3

1-Heptanol at 298.15 K, 10^4x_1 = 10.8 [65].

Cyclohexanol at 299.15 K, 10^4x_1 = 8.55 [81].

[a] Coefficients in eq (5).

[b] Standard deviation.

[c] Numbers of data points used.

[d] See text for references for each solvents.

K. Both Metschl's value[83] and Makranczy *et al.*'s value[80] at 298.15 K were omitted; they are lower than the smoothed value by 12% and 25%, respectively.

2-Propanol: Only the values of Kretschmer *et al.* at 273.15, 298.15, and 323.15 K[37] are available.

1-Butanol: The smoothed solubility values are based on the Kreschmer *et al.* data.[37] The Makranczy *et al.* value at 298.15 K[89] (which is 27% lower than Kreschmer *et al.*) was ignored.

2-Methyl-1-propanol: Only Battino *et al.* data are available, 274.09 to 327.96 K.[84]

1-Heptanol: Solubility data are available only at 298.15 K. The Ijams' value[65] is preferred to that of Makranczy *et al.*[89] in view of the trends in solubility with alcohol carbon number.

1-Octanol: The values of Wilcock *et al.* at 283.35 and 298.13 K,[72] Ijams at 298.15 K,[65] and Makranczy *et al.* at 298.15 K[89] are in satisfactory agreement. However, only the values of Wilcock *et al.* were used to obtain smoothed values.

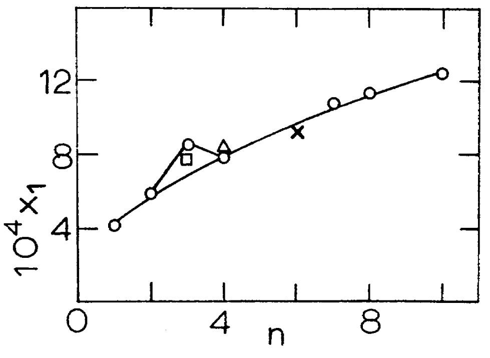

FIGURE 2. Smoothed mole fraction solubilities of oxygen at 101.325 kPa partial pressure of gas in 1-alkanols (circles) at 298.15 K. The square is for 2-propanol, the triangle for 2-methyl-1-propanol, and the cross is for cyclohexanol.

1-Decanol: The smoothed values are based on the values of Wilcock *et al.* at 282.74, 298.10, and 313.56 K.[72] The value of Makranczy *et al.* at 298.15 K[89] is 22% lower than that of Wilcock *et al.* at the same temperature and was rejected.

Cyclohexanol: Only Cauquil reports a value at 299.15 K.[81]

4.6.b. Ketones, Ethers, Acids, and Esters

For 2-propanone (acetone), 1,1-oxybisethane (diethyl ether), and acetic acid, methyl ester (methyl acetate), solubilities have been measured over a wide range of temperature (194.8 to 318 K). Smoothed solubility values for these three solvents are shown in Table 19. The solubility shows a minimum as a function of temperature for each of the solvents. Smoothed values for other ketones are shown in Table 20. For ketones, the solubility increases as a function of the carbon number, i.e., from 8.40×10^{-4} for 2-propanone to 11.74×10^{-4} for 2-hexanone at 298.15 K. Mole fraction solubility in noncyclic ethers ($10^4x_1 = 19$ at 298.15 K for 1,1-oxybisethane and 1,1-oxybispropane) is as high as those in normal alkanes. The solubility in cyclic ethers is about one-half of the values in normal alkanes. Some data for the solubility of oxygen in several ethers and an ester are given in Table 21.

The following summarizes the data treatment.

2-Propanone (acetone): Nine values of Horiuti, 194.85 to 313.15 K[73]; three values of Kretschmer *et al.*, 248.15 to 298.15 K[67]; and 21 values of Bub and Hillebrand, 298.2 to 318 K[85] are in satisfactory agreement. All of the data of the three groups except for seven points from Bub and Hillebrand, were used to obtain smoothed values. Metschl's value at 298.15 K[83] is 21% lower than the smoothed value and was omitted.

1,1-Oxybisethane (diethyl ether): Six values of Horiuti, 195.05 to 293.15 K,[73] a value of Schlapfer *et al.* at 293 K,[74]

Table 19. The mole fraction solubility of oxygen in 2-propanone(acetone); 1,1-oxybisethane(diethyl ether); and acetic acid, methyl ester(methyl acetate) at 101.325 kPa partial pressure of gas (10^4x_1)

T/K	2-Propanone (Acetone)	1,1-Oxybis-ethane (Diethyl ether)	Acetic acid, methyl ester (Methyl acetate)
193.15	8.718	25.90	8.326
203.15	8.442	24.02	8.226
213.15	8.250	22.61	8.175
223.15	8.124	21.55	8.166
233.15	8.051	20.77	8.191
243.15	8.021	20.19	8.244
253.15	8.029	19.78	8.322
263.15	8.068	19.52	8.421
273.15	8.134	19.36	8.539
283.15	8.224	19.30	8.674
293.15	8.336	19.33	8.824
298.15	8.399	19.37	8.905
303.15	8.466		8.988
313.15	8.614		9.165
323.15	8.778		
$A_o{}^a$	-12.1459	-13.2264	-10.8939
$A_1{}^a$	6.4940	9.7090	4.6602
$A_2{}^a$	2.6414	3.4083	2.1119
$10^4\sigma^b$	0.047	0.23	0.028
$\#^c$	27	8	10

[a] Coefficients in eq (5).
[b] Standard deviation.
[c] Number of data points used.
[d] See text for references for each solvent.

and a value of Christoff at 273.15 K[86] are in satisfactory agreement. The smoothed values are based on these values.

Acetic acid, methyl ester (methyl acetate): Nine values of Horiuti 194.75 to 313.15 K,[73] and a value of Schlapfer *et al.* at 293 K[74] are in satisfactory agreement and were used to obtain the smoothed values.

2-Butanone, 2-Pentanone, 2-Hexanone: Only Bub and Hillebrand's data are available.[85] All of the data were used to obtain smoothed values for each solvent.

Cyclohexanone: Only Guerry's data are available.[62]

1,1-Oxybispropane (dipropyl ether); tetrahydrofuran; 1,4-dioxane; tetrahydro-2H-pyran; acetic acid, ethyl ester (ethyl acetate): Only one group reports solubility values for each solvent except for 1,4-dioxane where Guerry's value[62] is 16% lower than the value of Schlapfer *et al.*[74] at 293.15 K.

Table 20. The mole fraction solubility of oxygen in four ketones at 101.325 kPa partial pressure of gas (10^4x_1)

T/K	2-Butanone	2-Pentanone	2-Hexanone	Cyclohexanone
293.15				6.38
298.15	10.11	11.12	11.74	6.36
303.15	10.20	11.16	11.67	
313.15	10.36	11.23	11.53	
323.15	10.52	11.30	11.40	
333.15	10.67	11.37	11.28	
343.15		11.43	11.17	
$A_o{}^a$	-6.3872	-6.5908	-7.1302	
$A_1{}^a$	-1.5186	-0.6285	1.1419	
$10^4\sigma^b$	0.13	0.13	0.17	
$\#^c$	20	22	22	2

[a] Coefficients in eq (5).
[b] Standard deviation.
[c] Number of data points used.
[d] See text for references for each solvents.

Table 21. The mole fraction solubility of oxygen in five oxygen containing solvents at 101.325 kPa partial pressure of gas (10^4x_1)

T/K	1,1-Oxybis-propane (Dipropyl ether)	Tetrahydro-furan	1,4-Dioxane	Tetrahydro-2H-pyran	Acetic acid, ethyl ester (Ethyl acetate)
293.15	18.8[a]	8.03[a]	5.20[a],6.16[b]	9.41[a]	8.70[b]
298.15	19.1[a]	8.16[a]	5.38[a]	9.64[a]	

[a] Guerry [62].
[b] Schlapfer, et al. [74].

4.7. Oxygen in Organic Compounds Containing Halogen

Smoothed values of mole fraction solubilities are shown in Table 22 as a function of temperature. The enthalpy of solution is nearly zero for carbon tetrachloride, positive for chlorobenzene ($\Delta\bar{H}_1^\circ = -973$ to -489 J mol^{-1} at 298.15 K), and negative for the perfluorocompounds (including perfluorotributylamine in Table 24: $\Delta\bar{H}_1^\circ = -973$ to -2313 J mol^{-1} at 298.15 K). For most of the solvents the solubility was measured only at 298.15 K. These data are shown in Table 23.

The following is a brief review of the original literature for the solvents listed in Table 21.

Table 22. Mole fraction solubility of oxygen in organic compounds containing halogen at 101.325 kPa partial pressure of gas (10^4x_1)

T/K	Carbon-tetra-chloride	Chloro-benzene	Hexafluoro-benzene	$C_8F_{16}O^a$ (FC-80)	$C_9F_{20}O^b$ (Caroxin-F)	$C_{10}F_{22}O_2{}^c$ (Caroxin-D)
273.15	12.02	7.780				
283.15	12.01	7.815	24.73			
293.15	12.00	7.859	24.36			
298.15	12.00	7.884	24.18	56.1	66.2	64.7
303.15	12.00	7.911		55.7	65.6	64.1
313.15	12.01	7.970		54.8	64.4	62.9
323.15	12.03	8.036		54.1	63.3	61.8
333.15	12.05	8.108				
343.15		8.184				
353.15		8.266				
$A_o{}^d$	-7.8804	-9.5100	-6.4518	-5.6610	-5.6147	-5.6434
$A_1{}^d$	1.6387	3.0621	1.2729	1.4255	1.7822	1.7995
$A_2{}^d$	0.5541	1.2243				
$10_4\sigma^e$	0.02	0.02	0.04	0.1	0.2	0.2
$\#^f$	7	9	4	5	5	5

[a] Heptafluorotetrahydro(nonafluorobutyl)furan or Perfluorobutylperfluorotetrahydrofuran.

[b] 1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluoro-6-[1,2,2,2,-tetrafluoro-1-(trifluoromethyl)ethoxy]-hexane or Perfluoro-1-isopropoxy hexane.

[c] 1,1,2,2,3,3,4,4-Octafluoro-1,4-bis[1,2,2,2-tetrafluoro-1-(trifluoromethyl)-ethoxy] butane or Perfluoro-1,4-diisopropoxy butane.

[d] Coefficients in eq (5).

[e] Standard deviation.

[f] Numbers of data points used.

[g] See text for references for each solvent.

Table 23. Mole fraction solubility of oxygen in organic compounds containing halogen at 298.15 K and 101.325 kPa partial pressure of gas

Solvent	10^4x	Solvent	10^4x_1
$C_3F_6Br_2$[a]	30.3[aa]	C_8F_{18}[k]	53.4[aa]
$C_6HF_{13}O$[b]	37.4[bb]	$C_9H_7F_{13}$[l]	49.4[bb]
Fluorobenzene	15.08[cc]	$C_9H_7F_{13}O$[m]	50.9[bb]
Bromobenzene	7.48[cc]	$C_9F_{19}Cl$[n]	51.1[aa]
Iodobenzene	5.10[cc]	C_9F_{20}[o]	53.5[aa]
1-Chlorohexane	13.5[dd]	$C_{10}H_9F_{13}$[p]	53.0[bb]
$C_7H_3F_{13}O$[c]	46.2[bb]	$C_{10}H_9F_{13}$[q]	50.2[bb]
1-Bromoheptane	13.2[ee]	$C_{10}F_{18}$[r]	39.0[aa]
$C_7F_{15}Br$[d]	47.5[aa]	$C_{11}HF_{23}O_3$[s]	68.3[aa]
$C_7F_{15}Cl$[e]	49.0[aa]	$C_{11}H_6F_{18}$[t]	47.8[bb]
C_7F_{14}[f]	45.6[aa]	$C_{11}F_{20}$[u]	40.6[aa]
C_7F_{16}[g]	55.5[ff]	$C_{12}F_{20}$[v]	42.0[aa]
$C_6H_4(CF_3)_2$[h]	63.1[aa]	$C_{14}HF_{29}O_4$[w]	75.9[aa]
$C_8H_5F_{13}O$[i]	51.4[bb]	$C_{17}HF_{35}O_5$[x]	85.3[aa]
$C_8F_{17}Br$[j]	56.6[aa]	$C_{29}HF_{59}O_9$[y]	118[aa]

[a] 1,2-Dibromo-1,1,2,3,3,3-hexafluoropropane.

[b] 1,1,1,3,3,4,4,5,5,5-Decafluoro-2-(trifluoromethyl)-2-pentanol.

[c] 1,1,1,2,2,3,3,5,5,5-Decafluoro-4-methoxy-4-(trifluoromethyl) pentane.

[d] 1-Bromo-1,1,2,2,3,3,4,4,5,6,6,6-dodecafluoro-5-(trifluoromethyl)-hexane.

[e] 1-Chloro-1,1,2,2,3,3,4,4,5,6,6,6-dodecafluoro-5-(trifluoromethyl) hexane.

[f] Undecafluoro(trifluoromethyl)cyclohexane or perfluoromethylcyclohexane

[g] Hexadecafluoroheptane or perfluoroheptane.

[h] Bis(trifluoromethyl)benzene.

[i] 2-Ethoxy-1,1,1,3,3,4,4,5,5,5-decafluoro-2-(trifluoromethyl)pentane.

[j] 1-Bromo-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane or perfluorooctylbromide.

[k] Octadecafluorooctane or perfluorooctane.

[l] 1,1,1,2,2,3,3-Heptafluoro-4,4-bis(trifluoromethyl)heptane.

[m] 1,1,1,2,2,3,3,5,5,5-Decafluoro-4-propoxy-4-(trifluoromethyl)pentane.

[n] 1-Chloro-1,1,2,2,3,3,4,4,5,5,6,6,7,8,8,8-hexadecafluoro-7-(trifluoromethyl)octane.

[o] Eicosafluorononane or perfluorononane.

[p] 1,1,1,2,2,3,3-Heptafluoro-4,4-bis(trifluoromethyl)octane.

[q] 1,1,1,2,2,3,3-Heptafluoro-6-methyl-4,4-bis(trifluoromethyl)-heptane.

[r] Octadecafluorodecahydronaphthalene or perfluorodecalin.

[s] 1,1,1,2,3,3-Hexafluoro-2-(heptafluoropropoxy)-3-[1,2,2-trifluoro-2-(1,2,2,2-tetrafluoroethoxy)-1-(trifluoromethyl)-ethoxy]propane.

[t] 1,1,1,7,7,7-Hexafluoro-2,2,6,6-tetrakis(trifluoromethyl)-heptane.

[u] Heptadecafluorodecahydro(trifluoromethyl)naphthalene or perfluoromethyldecalin.

[v] Tricycle[3.3.1.$1^{3,7}$]decane, tetradecafluorobis(trifluormethyl)-.

[w] 3,6,9,12-Tetraoxapentadecane, 1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,14,15,15,15-eicosafluoro-5,8,11-tris(trifluoromethyl)-.

[x] 3,6,9,12,15-Pentaoxaoctadecane, 1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,16,16,17,17,18,18,18-tricosafluoro-5,8,11,14-tetrakis(trifluoromethyl)-.

[y] 3,6,9,12,15,21,24,27-Nonaoxatriacontane, 1,1,1,2,4,4,5,7,7,8,10,10,11,13,13,14,16,16,17,19,19,20,22,22,23,25,25,26,28,28,29,29,30,30,30-pentacontafluoro-5,8,11,14,17,20,23,26-octakis(trifluoromethyl)-.

[aa] [88] [bb] [90] [cc] [76] [dd] [62] [ee] [65] [ff] [91]

Carbon tetrachloride: Horiuti[73] reports seven values over the temperature range of 273.15 to 333.15 K. The smoothed values were obtained from these values. Both values of Metschl[83] and Naumenko[61] at 298.15 K are lower than that of Horiuti by 19% and 17%, respectively.

Chlorobenzene: Nine values of Horiuti[73] over the temperature range of 273.15 to 353.15 K were used to obtain the smoothed values. The Naumenko *et al.*[76] point at 298.15 K is 14% higher than Horiuti's value at the same temperature.

Hexafluorobenzene: The smoothed values were obtained by using four values of Evans and Battino[87] in the temperature range between 282.92 and 297.81 K. The value of Wesseler *et al.*[88] at 298.15 K is 4.1% lower than that of Evans and Battino.

Perfluorobutylperfluorotetrahydrofuran; perfluoro-1-isopropoxy hexane; and perfluoro-1,4-diisopropoxy butane: Only the values of Tham *et al.* are available.[89]

4.8. Oxygen in Organic Compounds Containing Sulfur, Nitrogen, or Silicon

In most of the solvents, the solubility was reported only at 298.15 K. In pyrrolidine, pyridine, and piperidine, solubilities have been reported also at 293.15 K, but these differ by no more than 1.2% from the respective values at 298.15 K. Only for perfluorotributylamine and octamethylcyclotetrasiloxane are solubilities available for a wider temperature range. Smoothed values are given in Table 24. In dimethylsufloxide, two other groups report solubility values: Those of Baird and Foley[92] are 31% lower than that of Dymond[93]; Chaenko *et al.*[94] determined the solubility by using an electrochemical sensor and their value is 5.9 times higher than Dymond's value[93] when converted to 1 atm of oxygen partial

Table 24. Mole fraction solubility of oxygen in organic compounds containing sulfur, nitrogen, or silicon at 298.15 K at 101.325 kPa partial pressure of gas

Solvent	10^4x_1
Carbon disulfide	4.42[a]
Sulfinylbismethane (Dimethylsulfoxide)	1.57[b]
N-Methyl-N-nitroso-methanamine	2.00[c]
Pyrrolidine	6.06[d]
Pyridine	4.58[d]
Piperidine	7.35[d]
Nitrobenzene	4.95[e]
Benzeneamine (Aniline)	2.26[e]
N-Methylbenzeneamine	2.91[e]
2-Methylbenzeneamine	3.18[e]
3-Methylbenzeneamine	3.95[e]
N,N-Dimethylbenzeneamine	7.18[e]
N-Ethylbenzeneamine	7.66[e]
N,N-Diethylbenzeneamine	9.62[e]
Perfluorotributylamine(1,1,2,2,3,3,4,4,4-Nonafluoro-N,N-bis(nonafluorobutyl)-1-butanamine)	56.64 (273.15 K)[f]
	54.65 (293.15 K)[f]
	52.85 (293.15 K)[f]
	52.02[f]
	51.22 (303.15 K)[f]
Octamethylcyclotetrasiloxane	43.16 (293.15 K)[g]
	42.71[g]
	42.28 (303.15 K)[g]
	41.48 (313.15 K)[g]

[a] [91] [b] [93] [c] [92] [d] [62] [e] [76] [f] [66]

[g] Wilcock, R.J., McHale, J.L., Battino, R., and Wilhelm, E., Fluid Phase Equil. 2, 225 (1978).

pressure. For perfluorotributylamine, Wesseler *et al.*[88] and Zander[95] report solubility values, but only the Kobatake and Hildebrand values[66] were used to obtain the smoothed values. For nitromethane and 1-propyl nitrate, solubilities were reported by Chaenko *et al.*[94] and Amster and Levy,[96] but these are not included in Table 24.

4.9. Oxygen in Biological Fluids

Because of its biological importance the solubility of oxygen has been determined in many biological fluids. Some of these measurements are of reasonable precision, but a great many are of poor precision. Also, it is difficult to exactly characterize many of the biological fluids used. In terms of examining trends and having a rough knowledge of solubility, the data are reasonable. However, we will only report on two fluids here—solubilities in olive oil and in human blood. For the other fluids (including animal and vegetable oils, lipids and lipid solutions, aqueous protein solutions, serum plasma, tissue, alcoholic solutions, sugar solutions, and wines, among others) we refer you to Ref. 1.

4.9.a. Solubility in Olive Oil

The solubility of oxygen in olive oil has been determined by four groups,[97,29,98,99] but by far the most precise work was that done by Battino and co-workers.[99] Table 25 gives the smoothed mole fractions and Ostwald coefficients obtained from the following equation:

$$-[R/(\mathrm{J\ mol^{-1}\ K^{-1}})](T/\mathrm{K})\ln x_1 = 1240.9 + 39.809(T/\mathrm{K}). \qquad (22)$$

The density of olive oil is given by $\rho/(\mathrm{g\ cm^{-3}}) = 0.9152-0.000\,468\ (t/^\circ\mathrm{C})$ and its molecular weight is 884 ± 45 g mol^{-1}. The standard deviation of the solubility is about 0.5%.

Table 25. Smoothed values of the solubility of oxygen in olive oil at 101.325 kPa partial pressure of gas

T/K	Mole fraction 10^3x_1	Ostwald coeff. L
298.15	5.05	0.1269
308.15	5.13	0.1326
318.15	5.21	0.1383
328.15	5.29	0.1441

4.9.b. Solubility in Human Blood

The solubility of oxygen was determined in human blood of approximately 15.5 g/100 ml of hemoglobin by four groups.[28,100,101,102] There was substantial agreement and in the range 273 to 310 K their data can be represented by the following equation to about 4% for one standard deviation in the Bunsen coefficient:

$$\ln\alpha = 1.9685-0.018\,638(T/\mathrm{K}). \qquad (23)$$

At 310.15 K the smoothed value of the Bunsen coefficient is 0.0221.

4.10. Oxygen Solubility in Miscellaneous Fluids

See Ref. 1 for the solubility of oxygen in a variety of miscellaneous fluids. These data are not included here for the fluids are special, poorly characterized, or would need excessive space to fully characterize by physical properties. Included in the above-cited reference are solubilities in HF, SO_2, N_2O_4, $N_2 + CO_2$, mineral oil, oils, hydrocarbon fuels, petroleum, liquid paraffin, surfactants; and above 0.2 MPa solubilities in Cl_2, N_2O, and CO_2.

5. Ozone Solubilities

Except for the solubility of ozone in water, there are very few measurements of ozone solubilities. In this section we will only deal with the solubility of ozone in water. For solubilities of ozone in halogenated solvents, CCl_4 saturated with water and various concentrations of nitric acid, various concentrations of sulfuric acid, and a group of miscellaneous solvents (acetic acid, acetic anhydride, trifluoroacetic acid, methyl acetate, propionic acid, acetic acid/water mixtures, acetic acid + propionic acid, and ($Cl_4 + CHCl_2CHCl_2$ mixtures) see Battino.[1]

5.1. Ozone in Water

The determination of ozone solubilities in pure water is complicated because ozone decomposes irreversibly in water. The relevant presentation is

$$2O_3(g)\overset{1}{\rightleftarrows}2O_3(aq)\overset{2}{\rightleftarrows}3O_2(aq)\overset{3}{\rightleftarrows}3O_2(g). \qquad (24)$$

The relevant gas solubility is step 1, step 2 is irreversible, and step 3 may or may not attain equilibrium conditions. Unless extreme care is taken the solubility via step 1 may not be what is actually determined.

An analysis and solution of the problem is provided by Roth and his co-workers.[1,103,104] Their approach involved determining ozone concentrations in the gas phase in equilibrium with the ozone-saturated liquid (water) phase and doing this as a function of time so that the decomposition rate could also be determined. Since ozone solubility depends on the pH of the aqueous solution, solubilities were determined in buffered water, the pH being adjusted by

Table 26. Henry's Law constants for ozone solubilities in water at integer pH values and 276.15, 298.15 and 318.15 K using eq (25).

	$10^{-3}K_H$		
pH	276.15 K	298.15 K	318.15 K
1	2.18	3.92	6.03
2	2.36	4.24	7.08
3	2.56	4.60	7.68
4	2.78	4.99	8.32
5	3.01	5.41	9.02
6	3.26	5.86	9.78
7	3.54	6.35	10.60
8	3.83	6.88	11.49
9	4.15	7.46	12.45
10	4.50	8.09	13.50

H_2SO_4 or NaOH. In the temperature range 276.5 to 333.2 K (measurements also at 293.2 and 313.2 K) they found the following equation to best represent their data:

$$K_H = 3.842\times 10^7[OH^-]^{0.035}\exp[-2428/(T/K)]. \qquad (25)$$

K_H is the Henry's law constant [see Eq. (14)], and $[OH^-]$ is the hydroxide concentration in mol L^{-1}. The index of determination was 0.84 with a standard error at estimate of 0.20. Table 26 gives smoothed values obtained from Eq. (25) at three temperatures and at integral values of pH from 1 to 10. These values are considered to be the best currently available, but are necessarily of poor precision.

For a detailed discussion of other results of ozone solubility in water see Refs. 1, 103, and 104.

6. Concluding Observations

As befits its importance the solubility of oxygen has been measured in a wide variety of solvents and solutions. This paper shows some gaps in the coverage. Definitive studies need to be carried out in homologous series of n-alkanes and 1-alkanols over a range of temperatures. On the other hand, quite reliable values are now available for oxygen solubilities in water and seawater. Additional measurements are needed in heavy water, however.[105] For perspective we have prepared Fig. 3 which shows oxygen solubilities as a mole fraction at 101.325 kPa partial pressure of gas in some sixteen solvents as a function of temperature. Finally, if experimenters carried out their determinations over a wider range of temperatures, this would result in more reliable thermodynamic data.

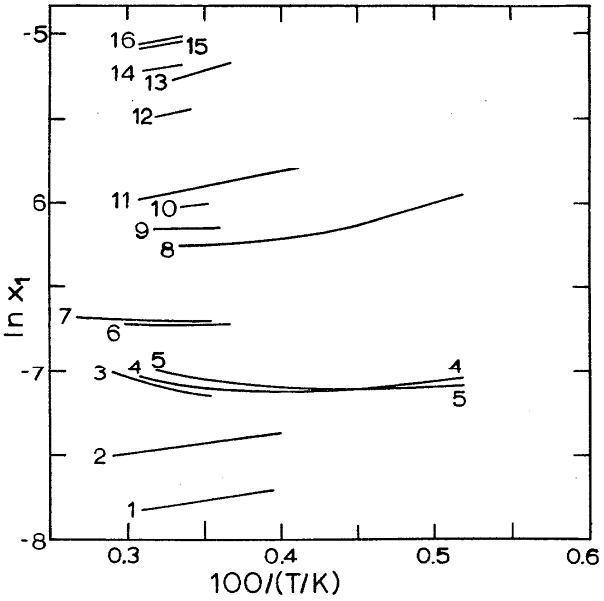

FIGURE 3. Mole fraction solubilities at 101.325 kPa partial pressure of oxygen in: 1—methanol; 2—ethanol; 3—benzene; 4—acetone; 5—methyl acetate; 6—carbon tetrachloride; 7—cyclohexane; 8—diethyl ether; 9—n-octane; 10—hexafluorobenzene; 11-2,2,4-trimethylpentane; 12—octamethylcyclotetrasiloxane; 13—perfluorotributylamine; 14—fluorocarbon fluid, FC-80; 15—caroxin-F; and 16—caroxin-D.

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8. References

[1] *Oxygen and Ozone*, IUPAC Solubility Data Series, edited by R. Battino (Pergamon, Oxford, 1981), Vol. 7.

[2] A. E. Markham and K. A. Kobe, Chem. Rev. **28**, 519 (1941).

[3] R. Battino and H. L. Clever, Chem. Rev. **66**, 395 (1966).

[4] H. L. Clever and R. Battino, "The Solubility of Gases in Liquids," in *Solutions and Solubilities*, edited by M. R. J. Dack (Wiley, New York, 1975), Vol. 8, Part 1, pp. 379–441.

[5] E. Wilhelm and R. Battino, Chem. Rev. **73**, 1 (1973).

[6] E. Wilhelm, R. Battino, and R. J. Wilcock, Chem. Rev. **77**, 219 (1977).

[7] W. Gerrard, *Solubility of Gases and Liquids* (Plenum, New York, 1976), p. 275.

[8] W. Gerrard, *Gas Solubilities, Widespread Applications* (Pergamon, Oxford, 1980), p. 497.

[9] A. S. Kertes, O. Levy, and G. Y. Markovits, "Solubility," in *Experimental Thermodynamics of Nonreacting Fluids*, Vol. II, edited by B. Vodar (Butterworth, London, 1975), pp. 725–748.

[10] *Solubilities of Inorganic and Organic Compounds*, edited by H. Stephen and T. Stephen, Vols. 1 and 2 (Macmillan, New York, 1963).

[11] A. Seidell, *Solubilities of Inorganic and Metal Organic Compounds*, 3rd ed. (Van Nostrand, New York, 1940).

[12] Landolt-Börnstein, 2. Teil, Bandteil b, *Lösungsgleichgewichte I* (Springer, Berlin, 1962); IV. Band, Technik, 4. Teil, Warmetechnik, Bandteil C, *Gleichgewicht der Absorption von Gasen in Flussigkeiten* (Springer, Berlin, 1976).

[13] *International Critical Tables*, edited by E. W. Washburn (McGraw-Hill, New York, 1926).

[14] J. M. Prausnitz, *Molecular Thermodynamics of Fluid-Phase Equilibrium* (Prentice-Hall, Englewood Cliffs, New Jersey, 1969), p. 523.

[15] J. H. Hildebrand, J. M. Prausnitz, and R. L. Scott, *Regular and Related Solutions* (Van Nostrand Reinhold, New York, 1970), p. 228.

[16] J. H. Dymond and E. B. Smith, *The Virial Coefficients of Pure Gases and Mixtures*, 2nd ed. (Clarendon, Oxford, 1980).

[17] B. B. Benson and D. Krause, J. Chem. Phys. **64**, 689 (1976).

[18] G. S. Kell, J. Chem. Eng. Data **15**, 119 (1970).

[19] B. B. Benson, D. Krause, and M. A. Peterson, J. Soln. Chem. **8**, 655 (1979).

[20] J. H. Carpenter, Limnol. Oceanog. **11**, 264 (1966).

[21] E. Douglas, J. Phys. Chem. **68**, 169 (1964).

[22] G. Geffcken, Z. Physik. Chem. **49**, 257 (1904).

[23] C. E. Klots and B. B. Benson, J. Marine Res. **21**, 48 (1963).

[24] J. Livingston, R. Morgan, and A. H. Richardson, J. Phys. Chem. **34**, 2356 (1930).

[25] C. N. Murray, J. P. Riley, and T. R. S. Wilson, Deep-Sea Res. **15**, 237 (1968).

[26] C. N. Murray and J. P. Riley, Deep-Sea Res. **16**, 311 (1969).

[27] D. M. Novak and B. E. Conway, Chem. Instrumentation **5**, 79 (1974).

[28] G. G. Power, J. Appl. Physiol. **24**, 468 (1968).

[29] G. G. Power and H. Stegall, J. Appl. Physiol. **29**, 145 (1970).

[30] H. A. Pray and E. F. Stephan, U.S. Atomic Energy Commission, BMI-840 (1953).

[31] H. Steen, Limnol. Oceanog. **3**, 423 (1958).

[32] W. Timofeev, Z. Physik. Chem. **6**, 141 (1890).

[33] E. L. Stephan, N. S. Hatfield, R. S. Peoples, and H. A. Pray, BMI-1067 (1956).

[34] H. A. Pray, L. E. Schweichert, and B. H. Minnich, Ind. Eng. Chem. **44**, 1146 (1952).

[35] H. L. Clever and C. H. Han, "The Solubility of Gases in Water from 350–600 K," in *Thermodynamics of Aqueous Systems with Industrial Applications*, ACS Symposium Series 133, edited by S. A. Newman (American Chemical Society, Washington, D.C., 1980), pp. 513–36.

[36] C. H. Mortimer, Internationale Vereinigung für Theoretische und Angewandte Limnologie, Communication No. 22, "The Oxygen Con-

tent of Air-saturated Fresh Waters over Ranges of temperature and Atmospheric Pressure of Limnological Interest," Stuttgart, 1981.

[37] R. F. Weiss, Deep-Sea Res. **17**, 311 (1970).

[38] C. T. Chen and J. H. Carpenter, unpublished manuscript (1978).

[39] D. J. J. Kinsman, M. Boardman, and M. Borcsik, in *4th Salt Symposium*, edited by A. H. Coogan (Northern Geological Society, Cleveland, Ohio, 1973), Vol. 1, p. 325.

[40] G. Bruhn, J. Gerlach, and F. Pawlek, Z. Anorg. Allg. Chem. **337**, 68 (1965).

[41] C. Bohr, Z. Physik. Chem. **71**, 47 (1910).

[42] V. L. Pogrebnaya, A. P. Usov, and A. V. Baranov, Zh. Vses. Khim. Obschchest. **17**, 344 (1972).

[43] N. E. Khomutov and E. I. Konnik, Zh. Fiz. Khim. **48**, 620 (1974).

[44] A. Broden and R. Simonson, Sven. Papperstidn. **81**, 541 (1978).

[45] A. Yasunishi, J. Chem. Eng. Jpn. **10**, 89 (1977); Kagaku Kogaku Rombunshu **4**, 185 (1978).

[46] S. K. Shoor, R. D. Walker, and K. E. Gubbins, J. Phys. Chem. **78**, 312 (1969).

[47] M. B. Knaster and L. A. Apel'baum, Zh. Fiz. Khim. **38**, 223 (1964); Russ. J. Phys. Chem. **38**, 120 (1964).

[48] G. G. MacArthur, J. Phys. Chem. **20**, 495 (1916).

[49] T. A. Mishnina, O. I. Avdeeva, and T. K. Bozhovskaya, Materialy Vses. Nauchn. Issled. Geol. Inst. **46**, 93 (1961).

[50] M. S. Guseva, E. I. Konnik, R. N. Sarti, A. A. Kuz'min, and I. L. Mordukhovich, Fiz. Khim. Rastvorov 105 (1972).

[51] K. A. Kobe and F. H. Kenton, Ind. Eng. Chem. Anal. Ed. **10**, 76 (1938).

[52] A.S. Jhaveri and M. M. Sharma, Chem. Eng. Sci. **23**, 1 (1968).

[53] A. Eucken and G. Hertzberg, Z. Physik. Chem. **195**, 1 (1950).

[54] T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655 (1955).

[55] R. I. Shkolinikova, Uch. Zap. Leningrad Gos. Univ., Ser. Khim. Nauk. Nr.**18**, 64 (1959).

[56] C. J. Anderson, R. A. Keeler, and S. J. Klach, J. Chem. Eng. Data **7**, 290 (1962),

[57] J. Tokunaga, J. Chem. Eng. Data **20**, 41 (1975).

[58] R. W. Cargill, J. Chem. Soc. Faraday Trans. 1 **72**, 2296 (1976).

[59] J. Markranczy, K. Megyery-Balog, L. Rusz, and L. Patyi, Hung. J. Ind. Chem. **4**, 269 (1976).

[60] C. Blanc and M. Batiste, Bull. Cent. Rech. Pau-SNPA **4**, 235 (1970).

[61] K. K. Naumenko, Candidates's thesis, Leningrad, 1970.

[62] D. Guerry, Ph.D. thesis, Vanderbilt University, 1944.

[63] E. S. Thomsen and J. C. Gjaldbaek, Acta Chem. Scand. **17**, 127 (1963).

[64] R. J. Wilcock, R. Battino, and W. F. Danforth, J. Chem. Thermodyn. **10**, 817 (1978).

[65] C. C. Ijams, Ph.D. thesis, Vanderbilt University, 1941.

[66] Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**. 331 (1961).

[67] C. B. Kretschmer, J. Nowakowska, and R. Wiebe, Ind. Eng. Chem. **38**, 506 (1946).

[68] R. R. Baldwin and S. G. Daniel, J. Inst. Petrol. **39**, 105 (1953); J. Appl. Chem. (London) **2**, 161 (1952).

[69] E. Wilhelm and R. Battino, J. Chem. Thermodyn. **5**, 117 (1973).

[70] J. D. Wild, T. Sridhar, and O. E. Potter, Chem. Eng. J. **15**, 209 (1978).

[71] E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197 (1976).

[72] R. J. Wilcock, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **9**, 111 (1977).

[73] J. Horiuti, Sci. Papers Inst. Phys. Chem. Research (Tokyo) **17**, 125 (1931).

[74] P. Schlapfer, T. Audykowski, and A. Bukowiecki, Schweiz, Arch. Angew. Wiss. Tech. **15**, 299 (1949).

[75] J. E. Byrne, R. Battino, and W. F. Danforth, J. Chem. Thermodyn. **6**, 245 (1974).

[76] N. K. Naumenko, M. M. Mukhin, and V. B. Aleskovskii, Zh. Prikl. Khim. (Leningrad) **42**, 2522 (1969); J. Appl. Chem. **42**, 2376 (1969).

[77] J. L. R. Morgan and H. R. Pyne, J. Phys. Chem. **34**, 2045 (1930).

[78] L. R. Field, E. Wilhelm, and R. Battino, J. Chem. Thermodyn. **6**, 237 (1974).

[79] G. T. Fisher, J. Chem. Eng. Data **8**, 206 (1963). [See correction, *ibid.* **8**, 571 (1963)].

[80] J. Makranczy, L. Rusz, and K. Balog-Megyery, Hung. Ind. Chem. **7**, 41 (1979).

[81] G. Cauquil, J. Chim. Phys. **24**, 53 (1927).

[82] S. A. Shchukarev and T. A. Tolmacheva, Zh. Strukt, Khim. **9**, 21 (1968); J. Struct. Chem. **9**, 16 (1968).

[83] J. Metschl, J. Phys. Chem. **28**, 417 (1924).

[84] R. Battino, F. D. Evans, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **3**, 743 (1971).

[85] G. K. Bub and W. A. Hillebrand, J. Chem. Eng. Data **24**, 315 (1979).

[86] A. Christoff, Z. Physik. Chem. **79**, 456 (1912).

[87] F. D. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753 (1971).

[88] E. P. Wesseler, R. Iltis, and L. C. Clark, J. Fluorine Chem. **9**, 137 (1977).

[89] M. K. Tham, R. D. Walker, and J. Modell, J. Chem. Eng. Data **18**, 385 (1973).

[90] D. D. Lawson, J. Moacanin, K. V. Scherer, T. F. Terranova, and J. D. Ingham, J. Fluorine Chem. **12**, 221 (1978).

[91] J. Chr. Gjaldbaek, Acta Chem. Scand. **6**, 623 (1952).

[92] W. R. Baird and R. T. Foley, J. Chem. Eng. Data **17**, 355 (1972).

[93] J. H. Dymond, J. Phys. Chem. **71**, 1829 (1967).

[94] N. V. Chaenko, G. I. Sukhova, N. K. Naumenko, and I. A. Kedrinskii, Zh Fiz. Khim. **53**, 1189 (1979); Russ. J. Phys. Chem. **53**, 1133 (1979).

[95] R. Zander, Res. Exp. Med. **164**, 97 (1974).

[96] A. B. Amster and J. B. Levy, ARS J. **29**, 870 (1959).

[97] D. Davidson, P. Eggleton, and P. Foggie, Quart. J. Exptl. Physiol. **37**, 91 (1952).

[98] P. J. Ke and R. G. Ackman, J. Am. Oil. Chem. Soc. **50**, 429 (1973).

[99] R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).

[100] C. Christoforides and J. Hedley-Whyte, J. Appl. Physiol. **27**, 592 (1969).

[101] F-J. W. Roughton and J. W. Severinghaus, J. Appl. Physiol. **35**, 861 (1973).

[102] C. Christoforides and J. Hedley-Whyte, J. Appl. Physiol. **40**, 815 (1976).

[103] D. E. Sullivan, Ph.D. Thesis, Vanderbilt University, 1979.

[104] J. A. Roth and D. E. Sullivan, Ind. Eng. Chem. Fundam. **20**, 137 (1981).

[105] *Note added in proof.* Cosgrove and Walkley just reported on the oxygen/D_2O system. Their data follow as temperature (T/K), and mole fraction solubility at 1 atm partial pressure of gas $\times 10^4$: 278.15, 0.3729; 283.15, 0.3332; 288.15, 0.2950; 293.15, 0.2673; 298.15, 0.2459; 303.15, 0.2263; 308.15, 0.2101; 313.15, 0.2000. B. A. Cosgrove and J. Walkley, J. Chromatog. **216**, 161 (1981).

[106] *Note added in proof.* See E. Wilhelm's article in *Nitrogen and Air*, in IUPAC Solubility Data Series edited by R. Battino (Pergamon, Oxford, 1982), Vol. 10, for a rigorous definition of the Ostwald coefficient particularly as applied to high precision measurements.