

COMPONENTS: (1) Ammonia; NH_3 ; [7664-41-7] (2) Organic liquids	EVALUATOR: P. G. T. Fogg, School of Chemistry, Polytechnic of North London, Holloway, London, U.K. January 1984
CRITICAL EVALUATION: <p>The solubility of ammonia has been measured in a wide variety of solvents. Some systems have been investigated by more than one worker or group of workers enabling comparisons between sets of results to be made. Comparison of solubilities in chemically similar solvents indicates general trends in solubility and draws attention to values which do not conform to general patterns. In cases where solubilities at several pressures have been measured the variation with pressure may be compared with that found for other systems. Where variations of solubility with change of temperature have been measured it is possible to compare the so-called "heats of solution" and "entropies of solution" for different systems. In cases where only a single solubility value at one temperature and one pressure has been measured the extent to which comparisons with other systems may be made, is rather limited.</p> <p>In some cases the solubilities of ammonia for given partial pressures have been reported. In other cases the solubilities correspond to given total pressures made up of partial pressures of solvent and partial pressures of ammonia. In order to compare different sets of measurements it has sometimes been necessary to convert solubility values for given total pressures to the corresponding mole fraction solubilities for a partial pressure of ammonia of 760 mmHg. In the absence of data from which activity coefficients can be calculated, approximate corrections have been made by the method used by Hildebrand (1). It has been assumed that the partial vapor pressure of the solvent is proportional to the mole fraction of the solvent (i.e., that the solvent obeys Raoult's law) and that the mole fraction solubility of ammonia is proportional to the partial pressure of ammonia over a short pressure range.</p> <p><u>Hydrocarbons</u></p> <p>In general, mole fraction solubilities are low compared with "Raoult's law" values and compared with mole fraction solubilities in alcohols measured under the same conditions. The solubilities are greater in aromatic hydrocarbons than in non-aromatic hydrocarbons.</p> <p><u>Non-aromatic hydrocarbons</u></p> <p>Hexane; C_6H_{14}; [110-54-3]</p> <p>Bell (2) measured the solubility of ammonia in hexane at 293.2 K and a partial pressure of 760 mmHg and also reported unpublished measurements of the mole fraction solubilities in octane, dodecane and hexadecane which had been measured by Brønsted and Volqvartz. The mole fraction solubility in hexane at 298.2 K and a partial pressure of 1 atm has been reported by Patyi <i>et al.</i> (3). If both solubility values for hexane are correct it would indicate a large variation of mole fraction solubility with change of temperature. This is not entirely inconsistent with the solubility data for amines in this solvent but both values should be used with caution.</p> <p>The Ostwald coefficient reported by Horsman-van den Dool and Warman (4) and measured at 292.4 K and an unspecified pressure can be compared with the solubility measurements discussed above if it is assumed that Ostwald coefficients are independent of pressure. The corresponding mole fraction solubility is about 7% less than the value at 298.2 K reported by Patyi <i>et al.</i> but Horsman-van den Dool and Warman used very simple apparatus.</p> <p style="text-align: right;">(cont.)</p>	

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<p>CRITICAL EVALUATION:</p> <p>Octane; C_8H_{18}; [111-65-9]; 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]; Dodecane; $\text{C}_{12}\text{H}_{26}$; [112-40-3]</p> <p>There are no other solubility values for octane and dodecane for direct comparison with the values reported by Bell. However Bell's value for the mole fraction solubility in octane at 293.2 K and 1 atm is within about 2% of the value for the mole fraction solubility in 2,2,4-trimethylpentane at 292.4 K and 1 atm which may be estimated from the Ostwald coefficient measured at an unspecified pressure by Horsman-van den Dool and Warman.</p> <p>Hexadecane; $\text{C}_{16}\text{H}_{34}$; [544-76-3]</p> <p>Tremper and Prausnitz (5) measured the solubilities of ammonia in hexadecane at eight temperatures between 300 K and 475 K. Henry's law constants were reported. The pressures at which measurements were made were not stated. Mole fraction solubilities at 1 atm calculated from these Henry's law constants are in agreement with the general pattern of data for the hydrocarbons. In particular, extrapolation of the mole fraction solubility at 1 atm to 293.2 K gives a value within about 8% of the mole fraction solubility of hexadecane at 1 atm as reported by Bell. The Henry's law constants measured by Tremper and Prausnitz are reliable for calculation of mole fraction solubilities to pressures of about 1 atm.</p> <p>The mole fraction solubilities in samples of kerosine and of diesel oil published by Messow and Pape (6) are in line with values for pure hydrocarbons of similar boiling point.</p> <p>Cyclohexane; C_6H_{12}; [110-82-7]</p> <p>The mole fraction solubility of ammonia in cyclohexane at 292.2 K and 1 atm from measurements by Kuznetsov <i>et al.</i> (7) is out of line with values for all other hydrocarbons and should therefore be disregarded.</p> <p>Ostwald coefficients for this system at unspecified pressures have been reported by Horsman-van den Dool and Warman (4) and also by Hentz and Sherman (8). In both cases very simple apparatus was used. Corresponding values of mole fraction solubilities for a partial pressure of 1 atm may be estimated on the assumption that Ostwald coefficients are independent of pressure. The Horsman-van den Dool value corresponds to a mole fraction solubility of about 0.011 at 1 atm and 292.5 K. The Hentz and Sherman value corresponds to a mole fraction of about 0.009 at 1 atm and about 297 K. Both of these values fall below the value of 0.035 at 1 atm and 298.2 K given by Patyi <i>et al.</i> (3). The apparatus and technique used by Patyi <i>et al.</i> are likely to be more reliable than those used by the other groups but further measurements on this system are needed in view of the disagreement between various solubility values.</p> <p>Methylcyclohexane; C_7H_{14}; [108-87-2]</p> <p>The Ostwald coefficient for solubility in methylcyclohexane at an unspecified pressure and 297.5 K has also been reported by Horsman-van den Dool and Warman. The value needs to be supported by other measurements on the system.</p> <p>1,1'-Bicyclohexyl; $\text{C}_{12}\text{H}_{22}$; [92-51-3]</p> <p>Mole fraction solubilities in 1,1'-bicyclohexyl at a partial pressure of 1 atm may be calculated from Henry's law constants measured by</p> <p style="text-align: right;">(cont.)</p>	

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<p>CRITICAL EVALUATION:</p> <p>Tremper and Prausnitz (5) at unspecified pressures and eight temperatures in the range 300 K to 475 K. These mole fraction solubilities are low compared with values for other hydrocarbons but may be accepted as reliable values. Horsman-van den Dool and Warman (4) have reported Ostwald coefficients for this system. These were measured at 295.6 K and 301.2 K and unspecified pressures and correspond to mole fraction solubilities which are over 20% greater than those which may be calculated from the Henry's law constants reported by Tremper and Prausnitz. The measurements by Horsman-van den Dool and Warman are likely to be less reliable than those carried out by Tremper and Prausnitz.</p> <p><i>cis</i>-Decahydronaphthalene; C₁₀H₁₈; [493-01-6]; <i>trans</i>-Decahydronaphthalene; C₁₀H₁₈; [493-02-7]</p> <p>Ostwald coefficients for solubilities of ammonia in <i>cis</i>- and <i>trans</i>-decalin were also measured by Horsman-van den Dool and Warman at 300.1 K and 301.3 K and unspecified pressures. The corresponding mole fraction solubilities may be estimated on the assumption that Ostwald coefficients are independent of pressure. These mole fraction solubilities are close to those estimated for 1,1'-bicyclohexyl from the Ostwald coefficients given by these authors for this compound and discussed above. Although no great reliance ought to be placed on these solubilities in the decalins until they are supported by other measurements on these systems, they are of the right order of magnitude.</p> <p>Cyclohexene; C₆H₁₀; 110-83-8</p> <p>The solubility of ammonia at 273.2 K and 293.2 K and various pressures in pure cyclohexene, in mixtures with benzene and in pure benzene have been measured by Noda <i>et al.</i> (9). The mole fraction solubilities in cyclohexene at 1 atm partial pressure, are lower than solubilities in alkanes or in benzene. The variation in solubility, as the proportion of cyclohexene is reduced, follows a consistent pattern. There is no reason to doubt the reliability of the measurements which can be accepted on a tentative basis.</p> <p><u>Aromatic hydrocarbons</u></p> <p>Benzene; C₆H₆; [71-43-2]</p> <p>Mole fraction solubilities are higher in aromatic hydrocarbons than in non-aromatic hydrocarbons. Mole fraction solubilities in benzene were measured by Noda <i>et al.</i> (9) at 273.2 K and 293.2 K and pressures approaching the vapor pressures of liquid ammonia at the temperatures of measurement. When these solubilities are plotted against the partial pressure of ammonia it is found that points fall on smooth curves which can be extrapolated through $x_{\text{NH}_3} = 1$; p_{NH_3} = vapor pressure of liquid ammonia.</p> <p>The mole fraction solubility at 293.2 K and a partial pressure of ammonia of 1 atm has been estimated from these measurements by the evaluator and found to be 0.038. This contrasts with the value of 0.0474 for this temperature and pressure given by Bell (2). The evaluator has also estimated the corresponding value at 298.2 K by extrapolation of values calculated from measurements by Noda <i>et al.</i> This estimated value of 0.033 also contrasts with the value of 0.0257 from work by Patyi <i>et al.</i> (3). Since the measurements by both Bell and Patyi <i>et al.</i> were made at one pressure only whereas the measurements reported by Noda <i>et al.</i> were made at a series of pressures and lead to a consistent set of solubility values, it is likely that the latter are</p> <p style="text-align: right;">(cont.)</p>	

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the most reliable. These should therefore be accepted as tentative values.

Methylbenzene; C₇H₈; [108-88-3]; 1-Methylnaphthalene; C₁₁H₁₀; [1321-94-4]

The mole fraction solubility in methylbenzene at 1 atm partial pressure of ammonia has been given by Bell (2) as 0.0313 at 293.2 K and by Gerrard (10) as 0.078 at 273.2 K. These values are similar in magnitude to values reported for the solubility of ammonia in benzene at the same temperatures and therefore the two values may be accepted as tentative values. However it would be unwise to extrapolate these values to obtain solubilities outside the range 273 K to 293 K. Henry's law constants for solubility in 1-methylnaphthalene are reliable for calculation of mole fraction solubilities to a pressure of about 1 atm.

Alcohols

The mole fraction solubility in alcohols and other compounds containing one or more -OH groups is high in comparison with the solubility in other liquids at the same temperature and partial pressure of ammonia. This may be due to the effect of hydrogen bonding between hydroxyl groups and nitrogen atoms in ammonia molecules. There is a general tendency for the mole fraction solubility in straight chain aliphatic alcohols to decrease with increase in length of the hydrocarbon chain. The mole fraction solubility is increased markedly if two or more hydroxyl groups are present in a solvent molecule. Ammonia has also a high solubility in chloro-substituted ethanols. This is consistent with a decrease of electron density at the oxygen atom with the replacement of hydrogen atoms by chlorine atoms.

Methanol; CH₄O; [67-56-1]

Solubilities at eight temperatures from 273.2 K to 313.2 K were determined by Hatem (11) at a total pressure equal to barometric pressure (unspecified). A single value at 291.2 K determined by Kuznetsov *et al.* (7) corresponds to a partial pressure of 1 atm. The values given by de Bruyn (12) for seven temperatures from 273.2 K to 301.6 K also correspond to a total pressure equal to barometric pressure as does the measurement by Delépine (13) at 273.2 K. Mole fraction solubilities at a partial pressure of 1 atm at three temperatures, corrected for the vapor pressure of the solvent and interpolated where necessary, are shown in Table 1. The single measurement by Delépine can be disregarded.

Table 1. Mole fraction solubilities of ammonia in methanol at $p_{\text{NH}_3} = 1$ atm from the results of several workers. Values have been interpolated and corrected for the vapor pressure of the solvent where necessary.

T/K	273.2	288.2	291.2
Hatem	0.49	0.35	0.33
de Bruyn	0.47	0.36	0.34
Kuznetsov <i>et al.</i>			0.35
Delépine	0.44		

(cont.)

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<p>CRITICAL EVALUATION:</p> <p>Considering the early date at which it was done, there is reasonable agreement between the work by de Bruyn and the later work by Hatem but the latter is likely to be the more reliable with better temperature control and probably better estimations of equilibrium concentrations. Kuznetsov <i>et al.</i> (7) were able to control temperatures to only ± 0.5 K. Poor temperature control may explain why the solubility measured at 291.2 K by these workers differs from the solubility reported by Hatem. There may also be differences in the way in which correction for the vapor pressure of the solvent has been made. It is recommended that the values given by Hatem, corrected to allow for the vapor pressure of the solvent, should be accepted as tentative values of the solubility at a partial pressure of 1 atm. These "corrected" values fit the equation:</p> $-RT \ln x_{\text{NH}_3} = -11570 + 48.68(T/K).$ <p>The use of this equation outside the range 273.2 K to 313.2 K is not recommended.</p> <p>Ethanol; C₂H₆O; [64-17-5]</p> <p>There is great discrepancy between the solubilities given by different workers. Barclay and Butler (14) carried out measurements at partial pressures of ammonia of about 10 mmHg. Extrapolation of these measurements to 760 mmHg is unlikely to give reliable estimation of solubility at this pressure and comparison with solubilities measured at 760 mmHg cannot be made. The solubility reported by Kuznetsov <i>et al.</i> (7) can be disregarded because the ethanol was only 92% pure. The purities of the ethanol used in the early work by Delépine (13) and in that by de Bruyn (12) were not stated but ethanol of high quality seems to have been used by Hatem (11). Values given by Hatem may therefore be more reliable than those reported by other workers even though the former do not conform to the general trend for monohydric straight-chain aliphatic alcohols. It should be noted, however, that ethanol shows a similar anomaly when the reported solubilities of diethylamine in various straight-chain alcohols are compared.</p> <p>1-Propanol; C₃H₈O; [71-23-8]</p> <p>Solubilities were measured by Hatem (11) at seven temperatures from 273.2 K to 308.2 K at a total pressure equal to barometric pressure. The interpolated value at 291.2 K, corrected for the vapor pressure of the solvent, differs by 8% from the single value obtained by Kuznetsov <i>et al.</i> (7) but the Hatem values can be tentatively accepted.</p> <p>2-Propanol; C₃H₈O; [67-63-0]</p> <p>Solubilities were also measured by Hatem (11) at seven temperatures from 273.2 K to 308.2 K at a total pressure equal to barometric pressure. The interpolated value at 291.2 K, corrected for the vapor pressure of the solvent, is close to the single value given by Kuznetsov <i>et al.</i> (7). The Hatem values can therefore be accepted as tentative values.</p> <p>1-Butanol; C₄H₁₀O; [71-36-3]</p> <p>Short <i>et al.</i> (15) measured solubilities in this solvent at three temperatures from 263.2 K to 333.2 K and a total pressure equal to 1 atm and corrected these measurements to give solubilities when the partial pressure of ammonia is 1 atm. The interpolated solubility at 273.2 K agrees with the value given by Maladkar (16) when the latter is corrected</p> <p style="text-align: right;">(cont)</p>	

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<p>CRITICAL EVALUATION:</p> <p>for the vapor pressure of the solvent. The solubility at 291.2 K interpolated from the values given by Short <i>et al.</i> is within 8% of the value given by Kuznetsov <i>et al.</i> The values of Short <i>et al.</i> can be accepted as reliable.</p> <p>2-Butanol; $\text{C}_4\text{H}_{10}\text{O}$; [78-92-2]</p> <p>Maladkar (16) measured the solubility at 273.2 K and a total pressure of 1 atm. The value obtained is lower than the corresponding value for 1-butanol just as values for 2-propanol are lower than values for 1-propanol. There is no reason to question the value given by Maladkar and it should be accepted as a provisional value.</p> <p>2-Methyl-1-propanol; $\text{C}_4\text{H}_{10}\text{O}$; [78-83-1]</p> <p>The single solubility measurement at 291.2 K and a partial pressure of 1 atm given by Kuznetsov <i>et al.</i> (7) is close to the value which they quote for 1-propanol. It should be borne in mind that temperature control was no better than ± 0.5 K and such an uncertainty in the temperature leads to an uncertainty in the mole fraction solubility quoted for 291.2 K of about ± 0.01.</p> <p>3-Methyl-1-butanol; $\text{C}_5\text{H}_{12}\text{O}$; [123-51-3]</p> <p>The mole fraction solubility calculated from measurements by Kuznetsov <i>et al.</i> (7) at the single temperature of 2-8.2 K and 1 atm is close to the value of the mole fraction solubility for 1-butanol under the same conditions. The solubility as measured by Kuznetsov can be accepted on a tentative basis with an estimated error in the mole fraction solubility of ± 0.01 due to uncertainty in the temperature.</p> <p>Octanol; $\text{C}_8\text{H}_{18}\text{O}$; [111-87-5]</p> <p>The value determined by Gerrard and Maladkar (10) at 273.2 K and a total pressure of 1 atm fits into the general pattern of results for aliphatic alcohols and can be accepted as a tentative value.</p> <p>Cyclohexanol; $\text{C}_6\text{H}_{12}\text{O}$; [108-93-0]</p> <p>The mole fraction solubility from work by Cauquil (17) at 299.2 K and 755 mmHg is about half the value for a straight-chain monohydric alcohol. In view of this and of the primitive nature of the apparatus which was used, the measurement should be used with great caution.</p> <p>2-Amino ethanol; $\text{C}_2\text{H}_7\text{NO}$; [141-43-5]</p> <p>The mole fraction solubility at 290.2 K and a partial pressure of 1 atm calculated from data published by Kuznetsov <i>et al.</i> (7) is lower than the solubility in ethanol under these conditions. This lower solubility is consistent with an increase in the electron density at the oxygen atom and with competition between amino groups and ammonia leading to a reduced tendency for hydrogen bonding to take place between oxygen and ammonia. The value can be accepted as a tentative value.</p> <p>1,2-Ethanedio1 (Ethylene glycol); $\text{C}_2\text{H}_6\text{O}_2$; [107-21-1]</p> <p>The solubility in this solvent at 263.2 K, 298.2 K and 333.2 K and a partial pressure of 1 atm were measured by Short <i>et al.</i> (15). Mole fraction solubilities are about twice the values for monohydric alcohols under the same conditions, showing the importance of the hydroxyl groups</p> <p>(cont.)</p>	

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CRITICAL EVALUATION:

in determining the solubility. The values for 298.2 K and 333.2 K lie close to the values of the mole fraction solubilities in diethylene glycol under the same conditions as calculated from data published by Timonin *et al.* (18). The measurements by Short *et al.* (15) therefore appear to be reliable and may be accepted as tentative values.

2,2'-Oxybisethanol (diethylene glycol); $\text{C}_4\text{H}_{10}\text{O}_3$; [111-46-6]

Measurements of solubilities in diethylene glycol were made by Timonin *et al.* (18) at four temperatures from 298.2 K to 343.2 K and pressures from 0.025 atm to 32.3 atm. As mentioned above, mole fraction solubilities for a pressure of 1 atm are close to values for ethylene glycol. The higher pressures reached are close to the vapor pressure of liquid ammonia. At temperatures above 298.2 K plots of x_{NH_3} against p_{NH_3} cross the reference line (line following Raoult's law). In terms of Raoult's law this means that there is a change from negative deviation to positive deviation as the pressure is increased. Such behavior has been reported for other systems and there seems to be no reason to doubt the measurements reported by Timonin *et al.* (18) which may be accepted as reliable values.

1,2,3-Propanetriol (glycerol); $\text{C}_3\text{H}_8\text{O}_3$; [56-81-5]

The mole fraction solubility at 291.2 K and a partial pressure of ammonia of 1 atm may be calculated from the mole ratio solubility given by Kuznetsov *et al.* (7). The value is close to that for ethylene glycol and for diethylene glycol under the same conditions with little apparent change in the solubility due to the presence of the extra hydroxyl group. However there is no reason to question the value which should be accepted on a tentative basis.

Chloroethanols

2-Chloroethanol; $\text{C}_2\text{H}_5\text{ClO}$; [59826-67-4]:
 2,2-Dichloroethanol; $\text{C}_2\text{H}_4\text{Cl}_2\text{O}$; [598-38-9]:
 2,2,2-Trichloroethanol; $\text{C}_2\text{H}_3\text{Cl}_3\text{O}$; [115-20-8]

Replacement of hydrogen atoms in the methyl group of ethanol by chlorine atoms is likely to reduce the electron density on the oxygen atom and hence increase the tendency towards hydrogen bonding between oxygen and dissolved ammonia. Measurements of solubilities at 273.2 K and a total pressure of 1 atm have been reported by Gerrard and Maladkar (10). Mole fraction solubilities are greater than the value for ethanol under the same conditions and are close to the value for ethylene glycol and for diethylene glycol. There is also an increase in the mole fraction solubility with increase in the number of chlorine atoms which one would expect. Values should be accepted on a tentative basis because they fit in with the general pattern of solubility data.

Other compounds containing oxygen

2-Propanone; $\text{C}_3\text{H}_6\text{O}$; [67-64-1]:
 Cyclohexanone; $\text{C}_6\text{H}_{10}\text{O}$; [108-93-0]

Careful measurements of the solubility of ammonia in acetone at 1 atm and temperatures of 263.2 K and 298.2 K have been carried out by Short *et al.* (15). The interpolated value of the mole fraction solubility at 292.2 K is 0.096 compared with the value of 0.28 calculated from measurements by Kuznetsov *et al.* (7) at this temperature. The dis-

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<p>CRITICAL EVALUATION:</p> <p>crepancy could be due to chemical reaction between acetone and ammonia during Kuznetsov's measurement. The measurements by Short <i>et al.</i> are likely to be the more reliable. Kuznetsov <i>et al.</i> (7) have also given a value for the solubility of ammonia in cyclohexanone but this has not been compiled because the formation of a solid precipitate was mentioned.</p> <p>1-Methyl-2-pyrrolidinone; $\text{C}_5\text{H}_9\text{NO}$; [872-50-4]</p> <p>The solubilities of ammonia in 1-methyl-2-pyrrolidinone at numerous temperatures and pressures have been reported by Freidson <i>et al.</i> (19). The measurements are self-consistent and there is no reason to doubt the reliability of the work.</p> <p>1,1'-Oxybisoctane; $\text{C}_{16}\text{H}_{34}\text{O}$; [629-82-3]</p> <p>The mole fraction solubility of ammonia in 1,1'-oxybisoctane (dioctyl ether) reported by Gerrard and Maladkar (10) is close to that for the mole fraction solubility in hydrocarbons of similar carbon number. There is no reason to doubt the value which may be accepted on a tentative basis.</p> <p>Acetic acid, octyl ester; $\text{C}_{10}\text{H}_{20}\text{O}$; [112-14-1]</p> <p>The solubility of ammonia in octyl acetate has also been measured by Gerrard and Maladkar (10). This value may also be accepted as a tentative value because there is again no reason to doubt its reliability.</p> <p>1,4-Dioxane; $\text{C}_4\text{H}_8\text{O}_2$; [123-91-1]</p> <p>The Ostwald coefficient for ammonia in 1,4-dioxane was measured at an unspecified pressure and about 297 K by Hentz and Sherman (8) but no great reliance can be placed on the value until it is supported by other measurements on the same system.</p> <p>Phosphorous acid, triphenyl ester; $\text{C}_{18}\text{H}_{15}\text{O}_3\text{P}$; [101-02-0]: Phosphorous acid, triethyl ester; $\text{C}_6\text{H}_{15}\text{O}_3\text{P}$; [122-52-1]: Phosphorous acid, dibutyl ester; $\text{C}_8\text{H}_{19}\text{O}_3\text{P}$:</p> <p>The solubilities in esters of phosphorous acid were studied by Maladkar (16). The measurements appear to be reliable and should be accepted on a tentative basis. The appreciable difference between the apparent mole fraction solubility in the dibutyl ester of phosphorous acid and that in the triethyl ester can be explained as being due to the presence of a free hydroxy group in the former solvent which is absent in the latter.</p> <p>Phosphoric acid, tributyl ester; $\text{C}_{12}\text{H}_{27}\text{O}_4\text{P}$; [126-73-8]</p> <p>The solubility of ammonia in tributyl phosphate was measured by Hála and Tuck (20) at 1 atm and several temperatures. The mole fraction solubility calculated from these measurements for 1 atm and 273.2 K is close to the value from measurements on the dibutyl ester of phosphorous acid reported by Maladkar (16). Measurements by Hála and Tuck can be accepted as tentative values.</p> <p style="text-align: right;">(cont.)</p>	

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<p>CRITICAL EVALUATION:</p> <p>1,2,3-Propanetriol, triacetate (glyceryl triacetate); $\text{C}_9\text{H}_{14}\text{O}_6$; [102-76-1]</p> <p>The mole fraction solubilities of ammonia in glyceryl triacetate, calculated from measurements by Furmer <i>et al.</i> (21) are similar in magnitude to values for solubilities in other esters. This work by Furmer <i>et al.</i> can also be accepted on a tentative basis.</p> <p>Triethoxysilane; $\text{C}_6\text{H}_{16}\text{O}_3\text{Si}$; [998-30-1]</p> <p>The mole fraction solubility of ammonia in triethoxysilane has been measured at various pressures and temperatures by Ditsent and Zolotareva (22). This is a consistent set of measurements which appear to be reliable and which should be accepted on a tentative basis.</p> <p><u>Chloro-compounds</u></p> <p>Tetrachloromethane; CCl_4; [56-23-5]: 1,2-Dichloroethane; $\text{C}_2\text{H}_4\text{Cl}_2$; [107-06-2]</p> <p>Bell (2) has given the mole fraction solubility in tetrachloromethane at 293.2 K and 1 atm partial pressure of ammonia as 0.0281. This value is close to values for aliphatic hydrocarbons. The value given by Bell for 1,2-dichloroethane under the same conditions is 0.0797. This increase can be explained as being due to a tendency for hydrogen bonding to occur between the hydrogen atoms of the solvent and the nitrogen atoms of the ammonia. There is no reason to question either the value given for tetrachloromethane or for 1,2-dichloroethane which may be accepted as tentative values.</p> <p>Trichloromethane; CHCl_3; [67-66-3]</p> <p>The solubility in trichloromethane was measured by Bell (2) at 293.2 K. The mole fraction solubility at a partial pressure of ammonia of 1 atm was reported to be 0.193. Seward (23) measured the solubility in this solvent at 298.2 K and at a pressure range from 14 mmHg to 453 mmHg. Extrapolation of Seward's results to 1 atm indicates a mole fraction solubility of 0.141 at 298.2 K and a partial pressure of ammonia of 1 atm. Hydrogen bonding between solvent and solute would be expected to lead to a high solubility of ammonia in trichloromethane but the apparent large change in solubility with a change of temperature from 293.2 K to 298.2 K must be viewed with caution and little reliance can be placed upon extrapolations to other temperatures.</p> <p>1-Chlorooctane; $\text{C}_8\text{H}_{17}\text{Cl}$; [111-85-3]</p> <p>The mole fraction solubility in 1-chlorooctane at 273.2 K and 1 atm has been measured by Gerrard and Maladkar (10). The value is greater than that for alkanes of similar chain length but less than that for trichloromethane. There is no reason to doubt the value which may be accepted as tentative.</p> <p>Chlorobenzene; $\text{C}_6\text{H}_5\text{Cl}$; [108-90-7]</p> <p>The solubility in chlorobenzene at 1 atm partial pressure of ammonia has been measured at 263.2 K, 298.2 K and 333.2 K by Short <i>et al.</i> (15). The interpolated value of the mole fraction solubility at 293.2 K is about 5% higher than the value reported by Bell (2) for this temperature.</p> <p style="text-align: right;">(cont.)</p>	

COMPONENTS:	EVALUATOR:
(1) Ammonia; NH ₃ ; [7664-41-7] (2) Organic liquids	P. G. T. Fogg, School of Chemistry, Polytechnic of North London, Holloway, London, U.K. January 1984
CRITICAL EVALUATION:	
The values reported by Short <i>et al.</i> are likely to be reliable. Comparison of these measurements with values for benzene reported by Noda <i>et al.</i> (9) shows that the introduction of a chlorine atom into the benzene nucleus may cause an increase in the mole fraction solubility. This would be consistent with the polarity of chlorobenzene.	
Bromobenzene; C ₆ H ₅ Br; [108-86-1]	
The mole fraction solubility of ammonia in bromobenzene was measured at 293.2 K by Bell (2) and the value for a partial pressure of 1 atm was reported. In this case the value is slightly less than the mole fraction solubility in benzene from Noda's measurements but the reliability of this single value for bromobenzene cannot be judged.	
Chloromethylbenzene; C ₇ H ₇ Cl; [100-44-7]	
Bell also reported the mole fraction solubility in chloromethylbenzene at 293.2 K and 1 atm partial pressure. The value appears to be greater than the corresponding values for benzene and for methylbenzene as would be expected from its polarity and there is no reason to question the value which may be accepted on a tentative basis.	
<u>Compounds containing nitrogen</u>	
Hydrazine; N ₂ H ₄ ; [302-01-2]: Methylhydrazine; N ₂ H ₃ CH ₃ ; [60-34-4]: 1,1-Dimethylhydrazine; N ₂ H ₂ C ₂ H ₆ ; [57-14-7]	
Mole fraction solubilities in hydrazine, methylhydrazine and 1,1-dimethylhydrazine were measured at three temperatures and several partial pressures of ammonia by Chang <i>et al.</i> (24). At each temperature, values of mole fraction solubilities, when plotted against the partial pressure of ammonia, fall on smooth curves through the origin and through $x_{\text{NH}_3} = 1$; $p_{\text{NH}_3} = \text{vapor pressure of liquid ammonia at the temperature of measurement}$. For each compound interpolated values of x_{NH_3} for $p_{\text{NH}_3} = 1$ atm fit closely to equations of the form:	
$-RT \ln x_{\text{NH}_3} = a + b(T/K).$	
There is no reason to doubt the reliability of these measurements.	
Benzenamine; C ₆ H ₇ N; [62-53-3]	
The mole fraction solubility in benzenamine (aniline) at a total pressure equal to barometric pressure and at six temperatures from 298.2 K to 423.2 K may be calculated from solubilities given by Stoica <i>et al.</i> (25). Extrapolation of these mole fraction solubilities to 291.2 K gives a value of 0.148 which may be compared with the value at this temperature given by Kuznetsov <i>et al.</i> (7) of 0.13. The vapor pressure of aniline made an appreciable contribution to the total pressure at the higher temperatures at which Stoica's measurements were carried out.	
If corrections are made for the vapor pressure of aniline then the mole fraction solubilities at a partial pressure of 1 atm from measurements by Stoica <i>et al.</i> may be accepted as tentative values. These values fit the equation:	

(cont.)

<p>COMPONENTS:</p> <p>(1) Ammonia; NH₃; [7664-41-7]</p> <p>(2) Organic liquids</p>	<p>EVALUATOR:</p> <p>P. G. T. Fogg, School of Chemistry, Polytechnic of North London, Holloway, London, U.K. January 1984</p>
<p>CRITICAL EVALUATION:</p> $-RT \ln x_{\text{NH}_3} = -25180 + 101.1(T/K)$ <p>(Standard deviation of $-RT \ln x_{\text{NH}_3} = 643 \text{ J mol}^{-1}$)</p> <p>This equation should be used with caution outside the range 298.2 K to 423.2 K.</p> <p><i>N,N</i>-Diethylethanamine (triethylamine); C₆H₁₅N; [121-44-8]</p> <p>The mole fraction solubility in triethylamine at 294.2 K and a partial pressure of ammonia of 1 atm may be calculated from measurements by Kuznetsov (7) to be 0.08. This is about half the value for the solubility in aniline at the same temperature. There is, however, no reason to doubt this value for triethylamine but there are no measurements on closely similar systems with which to make comparisons.</p> <p>Quinoline; C₉H₇N; [91-22-5]</p> <p>Kuznetsov <i>et al.</i> (7) have also made a single measurement of the solubility in quinoline at 291.2 K and 1 atm. The mole fraction solubility has been calculated to be 0.06, less than the value for triethylamine but slightly greater than the apparent value of 0.04 for benzene under the same conditions. The value for quinoline must be accepted as a tentative value because no proper evaluation can be carried out.</p> <p>Hexanedinitrile; C₆H₈N₂; [111-69-3]</p> <p>The solubility of ammonia in hexanedinitrile (adiponitrile) at several temperatures and pressures from about 70 mmHg to about 16 atm has been measured by Freidson <i>et al.</i> (26). These measurements correspond to a consistent set of values of mole fraction solubilities and seem to be reliable. However they should be accepted on a tentative basis because measurements on closely related systems are not available for comparison.</p> <p><u>Compounds containing silicon</u></p> <p>Tetramethylsilane; C₄H₁₂Si; [75-76-3]</p> <p>The Ostwald coefficient for dissolution of ammonia in tetramethylsilane was measured by Horsman-van den Dool and Warman (4) at 292.9 K and an unspecified pressure. The value is within the range found for dissolution in hydrocarbons but little reliance can be placed on this single value until other measurements on this or similar systems are available for comparison.</p> <p><u>References</u></p> <ol style="list-style-type: none"> Taylor, N. W.; Hildebrand, J. H. <i>J. Amer. Chem. Soc.</i> <u>1923</u>, 45, 682. Bell, R. P. <i>J. Chem. Soc.</i> <u>1931</u>, 1371. <p style="text-align: right;">(cont.)</p>	

COMPONENTS:	EVALUATOR:
<p>(1) Ammonia; NH₃; [7664-41-7]</p> <p>(2) Organic liquids</p>	<p>P. G. T. Fogg, School of Chemistry, Polytechnic of North London, Holloway, London, U.K. January 1984</p>
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