The mutual solubility of C_{5}–C_{26} hydrocarbons with seawater is exhaustively and critically reviewed. Reports of experimental determination of solubility in 46 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 15 of these systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. © 2006 American Institute of Physics. [DOI: 10.1063/1.2132316]

Key words: critical evaluation; hydrocarbons; seawater; solubility; water.
2.7. $o$-Xylene + Seawater. .......................... 799
2.8. $m$-Xylene + Seawater. .......................... 799
2.9. $p$-Xylene + Seawater. .......................... 800
2.10. Ethylbenzene + Seawater. ......................... 800
2.11. Octane + Seawater. ............................. 802
2.12. 1,2,3-Trimethylbenzene + Seawater. .......... 803
2.13. 1,2,4-Trimethylbenzene + Seawater. .......... 804
2.15. Cumene + Seawater. ............................ 805
2.16. Nonane + Seawater. ............................. 805
2.17. Naphthalene + Seawater. ......................... 806
2.18. Butylbenzene + Seawater. ....................... 810
2.19. sec-Butylbenzene + Seawater. .................. 810
2.20. tert-Butylbenzene + Seawater. ................. 811
2.21. Decane + Seawater. ............................ 811
2.22. 1-Methylnaphthalene + Seawater. .......... 813
2.23. Undecane + Seawater. ........................... 813
2.24. Acenaphthene + Seawater. ...................... 814
2.25. Biphenyl + Seawater*. ........................... 814
2.26. Dodecane + Seawater*........................... 816
2.27. Fluorene + Seawater. ........................... 818
2.28. Anthracene + Seawater. .......................... 818
2.29. Phenanthrene + Seawater* ....................... 820
2.30. Tetradecane + Seawater. ......................... 822
2.31. 2-Methylnaphthalene + Seawater. ........... 823
2.32. 1-Methylnaphthalene + Seawater. ........... 823
2.33. Fluoranthene + Seawater. ....................... 824
2.34. Pyrene + Seawater*. ............................. 824
2.35. Hexadecane + Seawater. ......................... 827
2.36. Benz[a]anthracene + Seawater. ............... 827
2.37. Chrysene + Seawater. ........................... 829
2.38. Octadecane + Seawater. ......................... 829
2.40. Benzo[e]pyrene + Seawater* .................. 830
2.41. Eicosane + Seawater. ........................... 832
2.42. Benzo[g,h,i]perylene + Seawater. .......... 832
2.43. Benzo[b]triphenylene + Seawater. .......... 833
2.44. Dibenzo[a,h]anthracene + Seawater. ....... 833
2.45. Dibenzo[a,j]anthracene + Seawater. ....... 834
2.46. Hexacosane + Seawater. ......................... 834
3. System Index ........................................... 835
4. Registry Number Index. ............................ 836
5. Author Index ......................................... 837

*A Critical Evaluation is prepared for this system

**List of Tables**

1. Experimental values for solubility of benzene (1) in seawater (2) .................. 788
2. Experimental values for solubility of hexane (1) in seawater (2). ................. 792
3. Experimental values for solubility of toluene (1) in seawater (2). .............. 794
4. Experimental values for solubility of heptane (1) in seawater (2). ............ 798
5. Experimental values for solubility of ethylbenzene (1) in seawater (2). ...... 800
6. Experimental values for solubility of octane (1) in seawater (2) ............... 802
7. Experimental values for solubility of naphthalene (1) in seawater (2) ....... 806
8. Experimental values for solubility of decane (1) in seawater (2). ............. 811
9. Experimental values for solubility of biphenyl (1) in seawater (2). .......... 814
10. Experimental values for solubility of dodecane (1) in seawater (2). ....... 816
11. Experimental values for solubility of anthracene (1) in seawater (2). ...... 818
12. Experimental values for solubility of phenanthrene (1) in seawater (2). .... 820
13. Experimental values for solubility of pyrene (1) in seawater (2). .......... 824
14. Experimental values for solubility of benz[a]anthracene (1) in seawater (2). 827
15. Experimental values for solubility of benzo[e]pyrene (1) in seawater (2). 830

**1. Preface**

1.1. Scope of this Volume

This paper is Part 12 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms. This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered). An exhaustive search of the primary chemical literature through the end of 2002 showed that no new measurements of solubility of hydrocarbons in seawater had been reported since the original review was completed. All new evaluations were prepared for this revision comparing experimental results for a given hydrocarbon seawater system to one another and to the related hydrocarbon water system. In these evaluations reported solubility values are characterized as “Recommended, Tentative, Doubtful, or Rejected,” based on consistency between independently determined experimental values. Recommended values are supported by two (or more) independent experimental values that agree within experimental precision and appear to be free of serious experimental problems. Tentative values are supported by two (or more) independent values in agreement with each other at a level slightly below that needed for a Recommended value or by a single value that is consistent with a Recommended value at nearby conditions of temperature or salinity. Experimental values that differ from other experimental values are Doubtful or Rejected.

A variety of units for the expression of solubility has appeared in the primary literature. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators. Where such conversions have been made, they are clearly attributed to the compiler and the source of any data not provided by the original investigators (e.g., hydrocarbon or seawater density) is specified. Defini-
tions of mass percent and mole fraction as well as their re-

ationship to other common measures of solubility are given

in the Introduction to this Volume.

The expression of the solubility of a hydrocarbon in natu-

ral seawater on a mole fraction basis presents special diffi-
culties since the composition of seawater is not fully known

and somewhat variable. However, the uncertainty introduced

by this factor is generally less than 3%, smaller than the

measurement uncertainty associated with many of the data.

Some data for hydrocarbon solubility in seawater have been
given in terms of the Setschenow (also transliterated from
the Russian as Sechenov and Setchenoff) equation. A de-
tailed discussion, “The Sechenov Salt Effect Parameter” has
appeared in press.3

Most measurements of hydrocarbon solubility in seawater
have been made in the temperature range considered “room

temperature” (275–300 K). In most reports system pressure

is unspecified but can be assumed to be approximately 100
kPa (1 atm). For most purposes this lack of specification of
system pressure is not important since hydrocarbon/water
solubilities do not vary strongly with pressure.

The editors wish to acknowledge the efforts compilers,
reviewers, and others whose careful work has contributed to

this paper.

1.2. References for the Preface

with Water and Seawater, Part I: Hydrocarbons C 5 to C 7 (Pergamon, New
York, 1989).

with Water and Seawater, Part II: Hydrocarbons C 8 to C 36 (Pergamon,

3. R. Battino, Editor, *IUPAC Solubility Data Series*, Vol. 10, Nitrogen and
2. Benzene+Seawater

2.2. Benzene

Critical Evaluation of Solubility of Benzene (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brown and Wasik¹</td>
<td>273–293</td>
<td>34.42</td>
</tr>
<tr>
<td>Mackay and Shiu²</td>
<td>298</td>
<td>0–200</td>
</tr>
<tr>
<td>May et al.³</td>
<td>298</td>
<td>0–40</td>
</tr>
<tr>
<td>Price⁴</td>
<td>298</td>
<td>1–360</td>
</tr>
</tbody>
</table>

Reference solubility data for benzene in pure water at 298 K were reported in Part 2 (Maczynski and Shaw⁶) and converted by the Evaluators to g (1/100 g sln).

The experimental data are listed in Table 1. At 298 K and a salinity of 34.47 and 35 g salts/kg sln, the values of Mackay and Shiu², May et al.³, and Price⁴ are in very good agreement. Each group of workers has also determined the solubility of toluene in pure water and obtained results within experimental error the reference value. Therefore, the mean of the reported values, 0.135 g (1/100 g sln), is accepted as Recommended at the indicated temperature and salinity. These studies measured solubility over range of salinities, Mackay and Shiu² reported their data in terms of the Setschenov equation. Their values may be used to interpolate solubilities at other salinities up to 200 g salt/kg sln.

Brown and Wasik¹ determined the solubility of benzene in seawater at a salinity of 34.42 g salt/kg sln over the temperature range 273–293 K. Linear extrapolation by the Evaluators of these results to 298 K gives a value 0.127 g (1/100 g sln). This suggests that the results of Brown and Wasik¹ may be slightly low and are Doubtful.

Rejected and Inaccessible Data

The data reported by Umano and Hayano⁵ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:


### Table 1. Experimental values for solubility of benzene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln)</th>
<th>Reference value for pure water g (1/100 g sln) ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>35</td>
<td>0.136 (R; mean from Refs. 2, 3, 4)</td>
<td>0.18 (R; mean from Refs. 2, 3, 4)</td>
</tr>
<tr>
<td>34.42 (Ref. 1)</td>
<td>0.128 (D; Ref. 1)</td>
<td>0.128 (D; Ref. 1)</td>
<td></td>
</tr>
<tr>
<td>35 (Ref. 2)</td>
<td>0.134 (R; Ref. 2)</td>
<td>0.134 (R; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>35 (Ref. 3)</td>
<td>0.1365 (R; Ref. 3)</td>
<td>0.1365 (R; Ref. 3)</td>
<td></td>
</tr>
<tr>
<td>35 (Ref. 4)</td>
<td>0.1391 (R; Ref. 4)</td>
<td>0.1391 (R; Ref. 4)</td>
<td></td>
</tr>
</tbody>
</table>
Components: (1) Benzene; C₆H₆; [71-43-2] (2) Artificial seawater

Variables: Prepared By:
Temperature: 0 – 20 °C
Salinity: 34.42 g salts/kg sln

G. T. Hefter and D. G. Shaw

- Variables: Prepared By:
  One temperature: 25 °C
  Salinity: 0–200 g (2) sln/kg sln

M. Kleinschmidt and W. Y. Shiu

Experimental Values

Solubility of benzene in water in artificial seawater

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 x₁ (compiler)</th>
<th>g (1)/100 g sln^a</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.19</td>
<td>3.129</td>
<td>0.1323 (0.0017)</td>
</tr>
<tr>
<td>5.32</td>
<td>3.255</td>
<td>0.1376 (0.0022)</td>
</tr>
<tr>
<td>10.05</td>
<td>3.186</td>
<td>0.1347 (0.0023)</td>
</tr>
<tr>
<td>14.96</td>
<td>3.117</td>
<td>0.1318 (0.0025)</td>
</tr>
<tr>
<td>20.04</td>
<td>3.065</td>
<td>0.1296 (0.0022)</td>
</tr>
</tbody>
</table>

^aNumbers in parentheses are standard deviations from 4 observations.

Experimental Values

The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation:

\[ \log \frac{S}{S_0} = K_S C_S \]

where
- \( S_0 \) is the solubility of \( \text{Benzene} \) in water (mg/L);
- \( S \) is the solubility of \( \text{Benzene} \) in solution (mg/L);
- \( K_S \) is the Setschenow constant (L/mol);
- \( C_S \) is the concentration of sodium chloride (L/mol);

evaluating the equation for \( S \) over the range of \( C_S \) 0–4 mol/L, \( K_S = 0.1836 \pm 0.0072 \) (standard error) with \( S_0 = 1779.5 \pm 16.4 \).

The corresponding mass percent and mole fraction, \( x_1 \), at salinity=35 g (2) sln/kg sln calculated by the compilers are 0.1340 g (1)/100 g sln and 3.227•10^-4 assuming a solution density of 1.025 kg/L.

Source and Purity of Materials:
(1) Research grade, 99.9% from Phillips Petroleum Co.
(2) and (3) Not specified.

Estimated Error:
Temperature: ±0.1 °C
Solubility: 95% confidence limit is about 8%.

Reference:

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor to avoid emulsification into a glass equilibrium cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:
(1) 99.9 mole % purity; source and methods of purification not specified.
(2) Prepared according to Sverdrup et al. Purity not specified.

Estimated Error:
Temperature: ±0.01 °C
Solubility: see table above.

References:

Experimental Values

Solubility of benzene in water in artificial seawater

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 x₁ (compiler)</th>
<th>g (1)/100 g sln^a</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.19</td>
<td>3.129</td>
<td>0.1323 (0.0017)</td>
</tr>
<tr>
<td>5.32</td>
<td>3.255</td>
<td>0.1376 (0.0022)</td>
</tr>
<tr>
<td>10.05</td>
<td>3.186</td>
<td>0.1347 (0.0023)</td>
</tr>
<tr>
<td>14.96</td>
<td>3.117</td>
<td>0.1318 (0.0025)</td>
</tr>
<tr>
<td>20.04</td>
<td>3.065</td>
<td>0.1296 (0.0022)</td>
</tr>
</tbody>
</table>

^aNumbers in parentheses are standard deviations from 4 observations.

Experimental Values

The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation:

\[ \log \frac{S}{S_0} = K_S C_S \]

where
- \( S_0 \) is the solubility of \( \text{Benzene} \) in water (mg/L);
- \( S \) is the solubility of \( \text{Benzene} \) in solution (mg/L);
- \( K_S \) is the Setschenow constant (L/mol);
- \( C_S \) is the concentration of sodium chloride (L/mol);

evaluating the equation for \( S \) over the range of \( C_S \) 0–4 mol/L, \( K_S = 0.1836 \pm 0.0072 \) (standard error) with \( S_0 = 1779.5 \pm 16.4 \).

The corresponding mass percent and mole fraction, \( x_1 \), at salinity=35 g (2) sln/kg sln calculated by the compilers are 0.1340 g (1)/100 g sln and 3.227•10^-4 assuming a solution density of 1.025 kg/L.

Source and Purity of Materials:
(1) Research grade, 99.9% from Phillips Petroleum Co.
(2) and (3) Not specified.

Estimated Error:
Temperature: ±0.1 °C
Solubility: 95% confidence limit is about 8%.

Reference:

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor to avoid emulsification into a glass equilibrium cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:
(1) 99.9 mole % purity; source and methods of purification not specified.
(2) Prepared according to Sverdrup et al. Purity not specified.

Estimated Error:
Temperature: ±0.01 °C
Solubility: see table above.

References:
### Experimental Values

The solubility of benzene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[
\log \frac{S_0}{S} = K S C_S
\]

where

- \(S_0\) is the solubility of benzene in water (mg/L);
- \(S\) is the solubility of benzene in solution (mg/L);
- \(K_S\) is the Setschenow constant (L/mol); and
- \(C_S\) is the concentration of sodium chloride (L/mol);

evaluating the equation for \(S\) over the range of \(C_S\) 0–0.7 mol/L, \(K_S\) = 0.175 with \(S_0\) = 1791.

The corresponding mass percent and mole fraction \(x_1\), at salinity = 35 g (2)kg sln calculated by the compilers are 0.1365 g (1)/100 g sln and 3.22 \(\times\) 10\(^{-4}\).

### Auxiliary Information

**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a generation column which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an extractor column packed with a superficially porous bonded C\(_{18}\) stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

### Source and Purity of Materials:

- **(1)** Greater than 97% pure.
- **(2)** Reagent grade.
- **(3)** Distilled from potassium–sodium hydroxide and passed through an XAD-2 column.

### Estimated Error:

**Temperature:** ± 0.05 °C.

\(K_S\) ± 0.006, \(S_0\) ± 10.

---

**Table:**

<table>
<thead>
<tr>
<th>Salinity (g/kg sln)</th>
<th>Experimental Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.96</td>
<td>0.1718 g (1)/100 g sln</td>
</tr>
<tr>
<td>3.78</td>
<td>0.1628 g (1)/100 g sln</td>
</tr>
<tr>
<td>3.28</td>
<td>0.1391 g (1)/100 g sln</td>
</tr>
<tr>
<td>2.85</td>
<td>0.1194 g (1)/100 g sln</td>
</tr>
<tr>
<td>1.48</td>
<td>0.0593 g (1)/100 g sln</td>
</tr>
<tr>
<td>1.01</td>
<td>0.0388 g (1)/100 g sln</td>
</tr>
<tr>
<td>0.581</td>
<td>0.0214 g (1)/100 g sln</td>
</tr>
<tr>
<td>0.378</td>
<td>0.0134 g (1)/100 g sln</td>
</tr>
</tbody>
</table>

---

### Notes:

1. Artificial seawater, composition not specified but probably similar to Lyman and Fleming.

### References:

Components:

(1) Benzene; C\textsubscript{6}H\textsubscript{6}; [71-43-2]
(2) Sodium Chloride; NaCl; [76-14-5]
(3) Water; H\textsubscript{2}O; [77-32-18-5]

Variables:

Temperature: 20–284 °C
Concentration of NaCl

Experimental Values

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10\textsuperscript{2} x\textsubscript{2} (compiler)</th>
<th>g (3/100 g sln)</th>
<th>Conc. NaCl\textsuperscript{a}</th>
</tr>
</thead>
<tbody>
<tr>
<td>281.0</td>
<td>63.29</td>
<td>28.46</td>
<td>0.0</td>
</tr>
<tr>
<td>271.5</td>
<td>59.21</td>
<td>25.11</td>
<td>0.0</td>
</tr>
<tr>
<td>250.1</td>
<td>47.41</td>
<td>17.22</td>
<td>0.0</td>
</tr>
<tr>
<td>223.0</td>
<td>29.95</td>
<td>8.98</td>
<td></td>
</tr>
<tr>
<td>186.0</td>
<td>16.7</td>
<td>4.42</td>
<td></td>
</tr>
<tr>
<td>78.0</td>
<td>0.103</td>
<td>0.240</td>
<td>9.939</td>
</tr>
<tr>
<td>66.0</td>
<td>0.814</td>
<td>0.189</td>
<td></td>
</tr>
<tr>
<td>40.0</td>
<td>3.29</td>
<td>0.0762</td>
<td></td>
</tr>
<tr>
<td>20.2</td>
<td>1.82</td>
<td>0.042</td>
<td></td>
</tr>
<tr>
<td>284.0</td>
<td>62.11</td>
<td>27.44</td>
<td>10.0</td>
</tr>
<tr>
<td>265.0</td>
<td>50.27</td>
<td>18.91</td>
<td></td>
</tr>
<tr>
<td>249.0\textsuperscript{b}</td>
<td>39.35</td>
<td>13.02</td>
<td></td>
</tr>
<tr>
<td>223.0\textsuperscript{c}</td>
<td>26.4</td>
<td>7.65</td>
<td></td>
</tr>
<tr>
<td>183.5</td>
<td>14.3</td>
<td>3.70</td>
<td></td>
</tr>
<tr>
<td>81.0</td>
<td>0.67</td>
<td>0.155</td>
<td>19.290</td>
</tr>
<tr>
<td>63.0</td>
<td>0.34</td>
<td>0.079</td>
<td></td>
</tr>
<tr>
<td>40.0</td>
<td>0.16</td>
<td>0.037</td>
<td></td>
</tr>
<tr>
<td>21.0</td>
<td>0.10</td>
<td>0.024</td>
<td></td>
</tr>
<tr>
<td>280.0</td>
<td>48.6</td>
<td>17.93</td>
<td>20.0</td>
</tr>
<tr>
<td>265.0</td>
<td>40.5</td>
<td>13.56</td>
<td></td>
</tr>
<tr>
<td>245.0</td>
<td>27.3</td>
<td>7.96</td>
<td></td>
</tr>
<tr>
<td>221.0</td>
<td>15.2</td>
<td>3.98</td>
<td></td>
</tr>
<tr>
<td>178.0</td>
<td>6.3</td>
<td>1.52</td>
<td></td>
</tr>
<tr>
<td>173.5</td>
<td>43.7</td>
<td>15.17</td>
<td></td>
</tr>
<tr>
<td>268.5</td>
<td>38.2</td>
<td>12.47</td>
<td></td>
</tr>
<tr>
<td>245.5</td>
<td>23.7</td>
<td>6.69</td>
<td></td>
</tr>
<tr>
<td>219.0</td>
<td>14.8</td>
<td>3.85</td>
<td></td>
</tr>
<tr>
<td>178.0</td>
<td>6.5</td>
<td>1.58</td>
<td></td>
</tr>
</tbody>
</table>

\textsuperscript{a}Stated as % in the paper: presumably g (2/100 g sln (compiler)).

\textsuperscript{b}Given as 294.0 in the original (corrected in personal communication by the authors to H. Miyamoto).

\textsuperscript{c}P = 54.23 atm.

Original Measurements:


Prepared By:

H. Miyamoto and G. T. Hefter

Auxiliary Information

Method/Apparatus/Procedure:

At higher temperatures (1) and the aqueous brine were placed in an autoclave, described in detail in the paper, and equilibrated by stirring. After settling, the solubility of (3) in (1) was determined volumetrically by withdrawing layers from the autoclave into a burette. At lower temperatures (1) and the aqueous solution were refluxed in a flask at constant temperature. After equilibration, an aliquot of the water rich layer was withdrawn and analyzed argentometrically and the solubility of (3) in (1) calculated. The solubility of NaCl in benzene was determined to be negligible in these experiments (8 \cdot 10\textsuperscript{-5} mol \cdot L\textsuperscript{-1} at 223 °C and 54.23 atm).

Source and Purity of Materials:

(1) C. P. grade; source not specified; purified by single fractional distillation.
(2) Not specified.
(3) C. P. grade; source not specified; recrystallized.

Estimated Error:

Not specified.
2.3. Methylcyclopentane+Seawater

Components:
(1) Methylcyclopentane, C₇H₁₂; [96-37-7]
(2) Sodium Chloride, NaCl; [7647-14-5]
(3) Water, H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C
Salinity: 1–360 g (±100 g)/sln

Prepared By:
M. Kleinschmidt and D. G. Shaw

Experimental Values
Solubility of methylcyclopentane in aqueous NaCl

<table>
<thead>
<tr>
<th>T/K</th>
<th>10^2 x_j (complex)</th>
<th>g (1/100 g sln)</th>
<th>g (2/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>8.14</td>
<td>0.00380</td>
<td>1.002</td>
</tr>
<tr>
<td></td>
<td>7.82</td>
<td>0.00563</td>
<td>10.000</td>
</tr>
<tr>
<td></td>
<td>6.40</td>
<td>0.00292</td>
<td>34.472*</td>
</tr>
<tr>
<td></td>
<td>5.98</td>
<td>0.00270</td>
<td>50.030</td>
</tr>
<tr>
<td></td>
<td>2.94</td>
<td>0.00127</td>
<td>125.100</td>
</tr>
<tr>
<td></td>
<td>1.38</td>
<td>0.000572</td>
<td>199.900</td>
</tr>
<tr>
<td></td>
<td>0.847</td>
<td>0.000336</td>
<td>279.800</td>
</tr>
<tr>
<td></td>
<td>0.495</td>
<td>0.000189</td>
<td>358.700</td>
</tr>
</tbody>
</table>

*Artificial sea water, composition not specified but probably similar to Lysand and Fleming.¹

References:

2.4. Hexane+Seawater

Components:
(1) Hexane, C₆H₁₄; [110-54-3]
(2) Seawater

Evaluators:
D. G. Shaw, Institute of Marine Science, University of Alaska,
Fairbanks, Alaska, USA.
A. Maczynski, Institute of Physical Chemistry, Polish Academy

Critical Evaluation of Solubility of Hexane (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author (s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquan-Yuen et al.¹</td>
<td>298</td>
<td>17.9–132.7</td>
</tr>
<tr>
<td>Freegarde et al.²</td>
<td>not specified</td>
<td>not specified</td>
</tr>
<tr>
<td>Krasnoshchekova and Gubergrits³</td>
<td>298</td>
<td>6</td>
</tr>
</tbody>
</table>

Reference solubility data for hexane in pure water at 298 K were reported in Part 4 (Maczynski and Shaw⁴) and converted by the Evaluators to g (1/100 g) sln.

The experimental data are listed in Table 2. Two determinations of Aquan-Yuen et al.¹ and Krasnoshchekova and Gubergrits³ were made at somewhat different salinities and thus cannot be directly compared. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergrits³ are Tentative. The data of Aquan-Yuen et al.¹ are Tentative.

Rejected and Inaccessible Data

The data reported by Freegarde et al.² lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

Table 2. Experimental values for solubility of hexane (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln) (T= tentative, D= doubtful)</th>
<th>Reference value for pure water g (1/100 g) sln ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>17.9 (Ref. 1)</td>
<td>1.035·10⁻³ (T= Ref. 1)</td>
<td>1.15·10⁻³</td>
</tr>
<tr>
<td></td>
<td>35.3 (Ref. 1)</td>
<td>7.86·10⁻⁴ (T= Ref. 1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>56.2 (Ref. 1)</td>
<td>7.25·10⁻⁴ (T= Ref. 1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>82.6 (Ref. 1)</td>
<td>4.60·10⁻⁴ (T= Ref. 1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>108.2 (Ref. 1)</td>
<td>3.47·10⁻⁴ (T= Ref. 1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>132.7 (Ref. 1)</td>
<td>2.32·10⁻⁴ (T= Ref. 1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6 (Ref. 3)</td>
<td>7.55·10⁻³ (D= Ref. 3)</td>
<td></td>
</tr>
</tbody>
</table>

Variables:
One temperature: 25 °C
Salinity: 110–130 g/kg sln.

Prepared By:
M. Aquan-Yuen, D. Mackay, and W. Y. Shiu

Experimental Values
Solubility of hexane in aqueous NaCl

<table>
<thead>
<tr>
<th>t°C</th>
<th>10^6 x</th>
<th>10^3 g (1/L) sln</th>
<th>g (2/L) sln^a</th>
<th>mol (2/L) sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.19</td>
<td>10.35</td>
<td>17.9</td>
<td>0.31</td>
</tr>
<tr>
<td>1.68</td>
<td>10.86</td>
<td>8.06</td>
<td>35.3</td>
<td>0.62</td>
</tr>
<tr>
<td>1.58</td>
<td>7.25</td>
<td>7.54</td>
<td>56.2</td>
<td>1.00</td>
</tr>
<tr>
<td>1.08</td>
<td>4.60</td>
<td>4.88</td>
<td>82.6</td>
<td>1.50</td>
</tr>
<tr>
<td>0.846</td>
<td>3.47</td>
<td>3.75</td>
<td>108.2</td>
<td>2.00</td>
</tr>
<tr>
<td>0.583</td>
<td>2.32</td>
<td>2.55</td>
<td>132.7</td>
<td>2.50</td>
</tr>
</tbody>
</table>

aCalculated by compiler.

M. Kleinschmidt and D. G. Shaw

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared by adding excess hexane (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 h and then allowed to settle for 48 h. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.


Variables:
One temperature: 25 °C
Salinity: 6 g/kg sln.

Prepared By:
M. Kleinschmidt

Experimental Values
The solubility of hexane in seawater was reported to be 7.55 \times 10^{-3} g (1/L) sln and the corresponding mole fraction, \( x_1 = 1.3 \times 10^{-5} \).

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

Source and Purity of Materials:
(1) “Chemically pure.”
(2) Distilled water plus salt mixture.

Estimated Error:
Not specified.
2.5. Toluene+Seawater

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brown and Wasik(^1)</td>
<td>273–293</td>
<td>34.42</td>
</tr>
<tr>
<td>Mackay and Shiu(^2)</td>
<td>298</td>
<td>0–200</td>
</tr>
<tr>
<td>Price(^3)</td>
<td>298</td>
<td>1–360</td>
</tr>
<tr>
<td>Rossi and Thomas(^4)</td>
<td>288–298</td>
<td>35</td>
</tr>
<tr>
<td>Sada et al.(^5)</td>
<td>298</td>
<td>29–108</td>
</tr>
<tr>
<td>Sutton and Calder(^6)</td>
<td>298</td>
<td>34.5</td>
</tr>
</tbody>
</table>

Reference solubility data for toluene in pure water at 298 K were reported in Part 5 (Maczynski and Shaw\(^7\)) and converted by the Evaluators to g (1/100 g sln). The experimental data are listed in Table 3. At 298 K and a salinity of 35 g salts/kg sln, the values of Mackay and Shiu\(^2\), Price\(^3\), and Sutton and Calder\(^6\) are in very good agreement. Each group of workers has also determined the solubility of toluene in pure water and obtained results within experimental error the reference value. Therefore, the mean of the reported values, 3.87 \times 10^{-2} g/l/100 g sln, is accepted as the Recommended value at the indicated temperature and salinity. Mackay and Shiu\(^2\) measured solubility over a range of salinities and reported their date in terms of the Setschenov equation. Their values may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

Brown and Wasik\(^1\) determined the solubility of toluene in seawater at a salinity of 34.42 salts/kg sln over the temperature range 273–293 K. Linear extrapolation by the Evaluators of these results to 298 K gives a value 3.80 \times 10^{-2} g/l/100 g. This suggests that the results of Brown and Wasik\(^1\) may be consistent with the Recommended value. The values reported by Sada et al.\(^5\) and Rossi and Thomas\(^4\) are in poorer agreement with the remaining data and are Doubtful.

References:

Experimental Values

Solubility of toluene in artificial seawater

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10^3 ( x_1 ) (compiler)</th>
<th>g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.19</td>
<td>9.0</td>
<td>0.0449 (0.0006)</td>
</tr>
<tr>
<td>5.32</td>
<td>8.60</td>
<td>0.0429 (0.0007)</td>
</tr>
<tr>
<td>10.05</td>
<td>8.34</td>
<td>0.0416 (0.0008)</td>
</tr>
<tr>
<td>14.96</td>
<td>8.12</td>
<td>0.0405 (0.0008)</td>
</tr>
<tr>
<td>20.04</td>
<td>7.96</td>
<td>0.0397 (0.0008)</td>
</tr>
</tbody>
</table>

*Numbers in parentheses are standard deviations from 4 observations.*

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor to avoid emulsification into a glass equilibration cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:
(1) 99.9 mole % purity; source and methods of purification not specified.
(2) Prepared according to Sverdrup et al. \(^1\) Purity not specified.

Estimated Error:
Temperature: ±0.03 °C
Solubility: see table above.

References:
### Toluene in Aqueous NaCl

**Experimental Values**

<table>
<thead>
<tr>
<th>Temperature ( ^\circ C )</th>
<th>( 10^3 \cdot x_1 ) (compiler)</th>
<th>g (1/100 g sln)</th>
<th>g (2/kg sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>10.3</td>
<td>0.0526</td>
<td>1.002</td>
</tr>
<tr>
<td>25</td>
<td>9.65</td>
<td>0.0490</td>
<td>10.000</td>
</tr>
<tr>
<td>25</td>
<td>8.04</td>
<td>0.0402</td>
<td>34.472*</td>
</tr>
<tr>
<td>25</td>
<td>7.26</td>
<td>0.0359</td>
<td>50.030</td>
</tr>
<tr>
<td>25</td>
<td>3.85</td>
<td>0.0182</td>
<td>125.100</td>
</tr>
<tr>
<td>25</td>
<td>2.34</td>
<td>0.0106</td>
<td>199.900</td>
</tr>
<tr>
<td>25</td>
<td>1.24</td>
<td>0.00538</td>
<td>279.800</td>
</tr>
<tr>
<td>25</td>
<td>0.890</td>
<td>0.00372</td>
<td>358.700</td>
</tr>
</tbody>
</table>

*Artificial seawater, composition not specified but probably similar to Lyman and Fleming.\(^1\)

### Solubility of Toluene in Seawater

**Experimental Values**

<table>
<thead>
<tr>
<th>Temperature ( ^\circ C )</th>
<th>( 10^3 \cdot x_1 )</th>
<th>g (1/100 g sln)</th>
<th>( \mu g (1)/g sln )</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>8.2</td>
<td>0.041</td>
<td>410</td>
</tr>
<tr>
<td>20</td>
<td>8.2</td>
<td>0.041</td>
<td>410</td>
</tr>
<tr>
<td>25</td>
<td>8.4</td>
<td>0.042</td>
<td>418.5</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Method/Apparatus/Procedure:**
  Saturate solution was prepared by equilibrating seawater with an excess of hydrocarbon for 24 h in a constant temperature gyroratory shaker followed by 12 h stationary period. A 100 ml aliquot was extracted three times with hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the hydrocarbon concentration.

- **Source and Purity of Materials:**
  - (1) From Burdick and Jackson, triple distilled in glass
  - (2) Collected off Scripps Pier and filtered twice through 0.22 \( \mu m \) membrane and twice extracted with hexane then its salinity adjusted to 35%.
  - (3) Hexane doubly distilled in glass.

- **Estimated Error:**
  - Temperature: ±0.1 °C.
  - Solubility: ±2%.

---

Components:
(1) Toluene; C₇H₈; [108-88-3]
(2) Sodium Chloride; NaCl; [7647-14-5]
(3) Water; H₂O; [7732-18-5]

Variables:
One temperature: 25 °C
Salinity: 29–108 g/100 g sln

Prepared By:
M. Kleinschmidt and D. G. Shaw

Experimental Values
Solubility of toluene in aqueous sodium chloride solutions

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10² x₁</th>
<th>g (1/100 g sln)</th>
<th>L (1/100 L sln)</th>
<th>g (2/100 g sln)</th>
<th>mol (2/100 L sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.95</td>
<td>0.0348</td>
<td>0.410</td>
<td>28.72</td>
<td>0.5011</td>
</tr>
<tr>
<td>5.06</td>
<td>0.0248</td>
<td>0.298</td>
<td>56.14</td>
<td>0.9991</td>
<td></td>
</tr>
<tr>
<td>3.76</td>
<td>0.0182</td>
<td>0.223</td>
<td>82.66</td>
<td>1.4933</td>
<td></td>
</tr>
<tr>
<td>2.87</td>
<td>0.0136</td>
<td>0.169</td>
<td>107.9</td>
<td>1.9933</td>
<td></td>
</tr>
</tbody>
</table>

*Calculated by compilers using density and other physical data for NaCl solutions from Weast and the assumption that the density of is 0.8669 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental apparatus and procedure used similar to those in Sobotka and Kahn. Toluene stained with 0.1% by weight. Sudan IV was added dropwise from a microburet into aqueous solution retained in a 1 L dissolution flask which was kept at 25.00 ± 0.01 °C in a thermostatically controlled water bath. The aqueous by a magnetic stirring device. Before saturation was reached, the Sudan IV was precipitated and floated on the surface as a solid. At saturation, the excess toluene appeared as immiscible red liquid droplets suspended in the aqueous solution. To ensure complete saturation, 24 h was allowed for equilibration.

Source and Purity of Materials:
(1) Reagent grade, source not specified.
(2) Reagent grade, source not specified.
(3) Not specified.

Estimated Error:
Solubility: 10⁻⁵ L (1/100 L sln.

References:
2.6. Heptane+Seawater

Components:
(1) Heptane; C₇H₁₆; [142-82-5]
(2) Seawater

Critical Evaluation of Solubility of Heptane (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freegarde et al.¹</td>
<td>not specified</td>
<td>not specified</td>
</tr>
<tr>
<td>Krasnoshchekova and Gubergrits²</td>
<td>298</td>
<td>6</td>
</tr>
</tbody>
</table>

Reference solubility data for heptane in pure water at 298 K were reported in Part 5 (Maczynski and Shaw³) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 4. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergrits² are considered Doubtful.

Rejected and Inaccessible Data

The data reported by Freegarde et al.¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

Experimental Values

The solubility of heptane in seawater was reported to be 1.03 x 10⁻³ g (1)/100 g sln and the corresponding mole fraction, x₁ = 1.9 x 10⁻³.

Source and Purity of Materials:
(1) “Chemically pure.”
(2) Distilled water plus salt mixture.

Estimated Error:
Not specified.

Method/Apparatus/Procedure:
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution.

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln (D=doubtful)</th>
<th>Experimental values g (1)/100 g sln</th>
<th>Reference value for pure water g (1)/100 g sln ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 2)</td>
<td>1.03 x 10⁻³ (D; Ref. 2)</td>
<td>2.95 x 10⁻⁴</td>
</tr>
</tbody>
</table>
### 2.7. o-Xylene + Seawater

**Components:**  
(1) o-Xylene: C₈H₁₀; [108-38-3]  
(2) Artificial seawater (Ref. 1)

**Original Measurements:**  

**Variables:**  
One temperature: 25.0 °C  
One salinity: 34.5 g salts/kg sln

**Prepared By:**  
M. Kleinschmidt

**Experimental Values**  
The solubility of o-xylene in artificial seawater is reported to be 129.6 mg/kg sln. The corresponding mass percent and mole fraction, \( x_1 \), calculated by the compiler are 0.01296 g/100 g sln and 2.26 \( \times 10^{-5} \) assuming the artificial seawater composition of Lyman and Fleming.¹

**Auxiliary Information**  

- **Method/Apparatus/Procedure:**  
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

- **Source and Purity of Materials:**  
  (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.
  (2) Made from doubly distilled water and salts 99+% pure.

- **Estimated Error:**  
  Temperature: ±0.1 °C  
  Solubility: 1.8 (standard deviation)

- **References:**  

### 2.8. m-Xylene + Seawater

**Components:**  
(1) m-Xylene: C₈H₁₀; [108-38-3]  
(2) Artificial seawater (Ref. 1)

**Original Measurements:**  

**Variables:**  
One temperature: 25.0 °C  
One salinity: 34.5 g salts/kg sln

**Prepared By:**  
M. Kleinschmidt

**Experimental Values**  
The solubility m-xylene in artificial seawater is reported to be 106.0 mg/kg sln. The corresponding mass percent and mole fraction, \( x_1 \), calculated by the compiler are 0.01060 g/100 g sln and 1.85 \( \times 10^{-5} \) assuming the artificial seawater composition of Lyman and Fleming.¹

**Auxiliary Information**  

- **Method/Apparatus/Procedure:**  
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

- **Source and Purity of Materials:**  
  (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.
  (2) Made from doubly distilled water and salts 99+% pure.

- **Estimated Error:**  
  Temperature: ±0.1 °C  
  Solubility: 0.6 (standard deviation)

- **References:**  
2.9. p-Xylene + Seawater

Components:
(1) p-Xylene; C₈H₁₀; [106-42-3]
(2) Artificial seawater

Variables:
One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln

Experimental Values
The solubility of p-xylene in artificial seawater is reported to be 110.9 mg/kg sln.

Critical Evaluation of Solubility of Ethylbenzene (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

References:

Table 5. Experimental values for solubility of ethylbenzene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln) (T=0.9 standard deviation)</th>
<th>Reference value for pure water g (1/100 g sln) ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>273</td>
<td>34.4</td>
<td>1.40 • 10⁻² (T; Ref. 1)</td>
<td>2.00 • 10⁻²</td>
</tr>
<tr>
<td>278</td>
<td>34.4</td>
<td>1.33 • 10⁻² (T; Ref. 1)</td>
<td>1.94 • 10⁻²</td>
</tr>
<tr>
<td>283</td>
<td>34.4</td>
<td>1.29 • 10⁻² (T; Ref. 1)</td>
<td>1.88 • 10⁻²</td>
</tr>
<tr>
<td>288</td>
<td>34.4</td>
<td>1.25 • 10⁻² (T; Ref. 1)</td>
<td>1.82 • 10⁻²</td>
</tr>
<tr>
<td>293</td>
<td>34.4</td>
<td>1.22 • 10⁻² (T; Ref. 1)</td>
<td>1.88 • 10⁻²</td>
</tr>
<tr>
<td>298</td>
<td>34.5</td>
<td>1.11 • 10⁻² (T; Ref. 2)</td>
<td>1.88 • 10⁻²</td>
</tr>
</tbody>
</table>
Components: (1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Artificial seawater


Variables: Prepared By: G. T. Hefter and D. G. Shaw

Temperature: 0 – 20 °C
Salinity: 34.42 g salts/kg sln

Experimental Values
Solubility of ethylbenzene in artificial seawater

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^3 x₁ (compiler)</th>
<th>g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.19</td>
<td>2.44</td>
<td>0.0140 (0.0002)</td>
</tr>
<tr>
<td>5.32</td>
<td>2.31</td>
<td>0.0133 (0.0003)</td>
</tr>
<tr>
<td>10.05</td>
<td>2.25</td>
<td>0.0129 (0.0003)</td>
</tr>
<tr>
<td>14.96</td>
<td>2.18</td>
<td>0.0125 (0.0003)</td>
</tr>
<tr>
<td>20.04</td>
<td>2.12</td>
<td>0.0122 (0.0003)</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 L of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities is not given.

Source and Purity of Materials:
(1) 99.99 mole % purity, source and methods of purification not specified.
(2) Prepared according to Sverdrup et al. Purity not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: see table above.

References:

Components: (1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Artificial seawater (Lyman and Fleming)


Variables: Prepared By: M. Kleinschmidt

One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln

Experimental Values
The solubility of ethylbenzene in artificial seawater is reported to be 111.0 mg (1/kg sln).
The corresponding mass percent and mole fraction, x₁, calculated by the compiler are 0.01110 g (1/100 g sln and 1.9 \times 10^{-5} assuming the artificial seawater composition of Lyman and Fleming.

Auxiliary Information

Method/Apparatus/Procedure:
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:
(1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1.3 (standard deviation).

References:
2.11. Octane+Seawater

**Components:**
(1) Octane; C₈H₁₈ [111-65-9]
(2) Seawater

**Evaluators:**
D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA

---

**Critical Evaluation of Solubility of Octane (1) in Seawater (2)**

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freegarde et al.¹</td>
<td>not specified</td>
<td>not specified</td>
</tr>
<tr>
<td>Krasnoschekova and Gubergrits²</td>
<td>298</td>
<td>6</td>
</tr>
</tbody>
</table>

Reference solubility data for octane in pure water at 298 K were reported in Part 7, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 6. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoschekova and Gubergrits² are considered Doubtful.

**Rejected and Inaccessible Data**

The data reported by Freegarde et al.¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

**References:**

---

**Experimental Values**

The solubility of octane was reported to be 1.0 mg/L. The corresponding mass percent and mole fraction (x₁), calculated by the compilers, are 1.0 \( \times 10^{-4} \) g (1)/100 g sln and 1.6 \( \times 10^{-5} \), respectively, assuming a solution density of 1.02 kg/L.

**Auxiliary Information**

<table>
<thead>
<tr>
<th>Method/Apparatus/Procedure:</th>
<th>Source and Purity of Materials:</th>
<th>Estimated Error:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None given except that analysis was done using gas chromatography.</td>
<td>Not given.</td>
<td>Not specified.</td>
</tr>
</tbody>
</table>

---

**Table 6. Experimental values for solubility of octane (1) in seawater (2)**

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1)/100 g sln (D=doubtful)</th>
<th>Reference value for pure water g (1)/100 g sln ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 2)</td>
<td>2.5 ( \times 10^{-4} ) (D; Ref. 2)</td>
<td>6.3 ( \times 10^{-5} )</td>
</tr>
</tbody>
</table>
2.12. 1,2,3-Trimethylbenzene + Seawater

**Components:**
1. 1,2,3-Trimethylbenzene; C₉H₁₂; [526-73-8]
2. Artificial seawater (Lyman and Fleming)

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Prepared By:**
- M. Kleinschmidt

**Experimental Values**
The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg/kg sln. The corresponding mass percent and mole fraction ($x₁$), calculated by the compiler, are $4.86 \times 10^{-3}$ g/100 g sln and $7.47 \times 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.

**Auxiliary Information**
- **Method/Apparatus/Procedure:**
  A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

- **Source and Purity of Materials:**
  1. From Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.
  2. Made from doubly distilled water and salts 99+% pure.

- **Estimated Error:**
  Temperature: ±0.1 °C.
  Solubility: 0.5 (standard deviation).

**References:**
### 2.13. 1,2,4-Trimethylbenzene + Seawater

**Components:**
- (1) 1,2,4-Trimethylbenzene, C₉H₁₂ [95-63-6]
- (2) Artificial seawater (Lyman and Fleming)

**Original Measurements:**

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Prepared By:**
M. Kleinschmidt

**Experimental Values**
The solubility of 1,2,4-trimethylbenzene in artificial seawater is reported to be 39.6 mg/kg sln.
The corresponding mass percent and mole fraction \((x_1)\), calculated by the compiler, are \(3.96 \cdot 10^{-3}\) g/100 g sln and \(6.09 \cdot 10^{-6}\), respectively, assuming the artificial seawater composition of Lyman and Fleming.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
- (2) Made from doubly distilled water and salts 99+ % pure.

**Estimated Error:**
- Temperature: ±0.1 °C.
- Solubility: 0.5 (standard deviation).

**References:**

### 2.14. Mesitylene + Seawater

**Components:**
- (1) Mesitylene, 1,3,5-trimethylbenzene, C₉H₁₂ [108-67-8]
- (2) Artificial seawater (Lyman and Fleming)

**Original Measurements:**

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Prepared By:**
M. Kleinschmidt

**Experimental Values**
The solubility of mesitylene in artificial seawater is reported to be 31.3 mg/kg sln.
The corresponding mass percent and mole fraction \((x_1)\), calculated by the compiler, are \(3.13 \cdot 10^{-3}\) g/100 g sln and \(4.81 \cdot 10^{-6}\), respectively, assuming the artificial seawater composition of Lyman and Fleming.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
- (2) Made from doubly distilled water and salts 99+ % pure.

**Estimated Error:**
- Temperature: ±0.1 °C.
- Solubility: 0.2 (standard deviation).

**References:**
### 2.15. Cumene + Seawater

**Components:**
1. Cumene (isopropylbenzene); C₉H₁₂; CAS 98-82-8
2. Artificial seawater (Lyman and Fleming)¹

**Original Measurements:**

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Experimental Values**
The solubility of cumene in artificial seawater is reported to be 42.5 mg (100 g sln).

**Auxiliary Information**
- **Method/Apparatus/Procedure:**
  A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

- **Source and Purity of Materials:**
  1. From either Aldrich Chemical Co. or Matheson Coleman and Bell. 99% pure.
  2. Made from doubly distilled water and salts 99% pure.

- **Estimated Error:**
  - Temperature: ±0.1 °C
  - Solubility: 0.5 (standard deviation).

- **References:**

### 2.16. Nonane + Seawater

**Components:**
1. Nonane; C₉H₂₀; CAS 111-84-2
2. Seawater

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 6 g/kg sln

**Experimental Values**
The solubility of nonane in seawater was reported to be 4.3 \times 10⁻³ g (100 g sln) and the corresponding mole fraction, \( x_1 = 6.0 \times 10⁻⁸ \).

**Auxiliary Information**
- **Method/Apparatus/Procedure:**
  A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

- **Source and Purity of Materials:**
  1. “Chemically pure.”
  2. Distilled water plus salt mixture.

- **Estimated Error:**
  Not specified.
### 2.17. Naphthalene + Seawater

#### Components:
- Naphthalene: C_{10}H_{8} \[91-20-3\]
- Seawater

#### Evaluators:
- D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

#### Critical Evaluation of Solubility of Naphthalene (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eganhouse and Calder</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Gordon and Thorne</td>
<td>298</td>
<td>31.7</td>
</tr>
<tr>
<td>Gordon and Thorne</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>May et al</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Paul</td>
<td>298</td>
<td>30.59</td>
</tr>
<tr>
<td>Schwarz</td>
<td>281–303</td>
<td>30</td>
</tr>
</tbody>
</table>

Reference solubility data for naphthalene in pure water at 298 K were reported in Part 9, Shaw and Maczynski,\(^7\) and converted by the Evaluators to g (1/100 g sln).

The experimental data are listed in Table 7. At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder, Gordon and Thorne, and May et al. are in good agreement. Therefore all these data and the mean value, 2.28 \(\times\) 10\(^{-3}\) are adopted as the Recommended value at this temperature and salinity. Since the value of Schwarz is lower than would be expected with decreasing salinity, it is considered Doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul and of Gordon and Thorne are in fair agreement. Therefore their data are adopted as Tentative values. Gordon and Thorne\(^2\) and May et al.\(^3\) report data for a range of salinities using the Sctchenow equation. Schwarz\(^6\) reports data over the temperature range 281–303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

#### References:

#### Table 7. Experimental values for solubility of naphthalene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln)</th>
<th>Reference value for pure water g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>35</td>
<td>2.28 (\times) 10(^{-3}) (R; mean from Refs. 1, 3, and 4)</td>
<td>± 30%</td>
</tr>
<tr>
<td>31.7</td>
<td>(Ref. 2)</td>
<td>2.47 (\times) 10(^{-3}) (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>(Ref. 3)</td>
<td>2.36 (\times) 10(^{-3}) (R; Ref. 3)</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>(Ref. 4)</td>
<td>2.29 (\times) 10(^{-3}) (R; Ref. 4)</td>
<td></td>
</tr>
<tr>
<td>30.59</td>
<td>(Ref. 5)</td>
<td>2.53 (\times) 10(^{-3}) (T; Ref. 5)</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>(Ref. 6)</td>
<td>4.76 (\times) 10(^{-3}) (D; Ref. 6)</td>
<td></td>
</tr>
</tbody>
</table>
### Experimental Values

**Natural seawater**

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>One temperature: 25 °C</td>
<td>W. Y Shiu and D. Mackay</td>
</tr>
<tr>
<td>Salinity: 10–32 g/kg sln</td>
<td></td>
</tr>
</tbody>
</table>

#### Solubility of naphthalene in natural seawater at 25 °C

<table>
<thead>
<tr>
<th>Salinity (g/kg sln)</th>
<th>Chlorosity (%)</th>
<th>Treatment</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.47</td>
<td>17.96</td>
<td>MF</td>
</tr>
<tr>
<td>3.45</td>
<td>17.96</td>
<td>GFF</td>
</tr>
<tr>
<td>3.49</td>
<td>18.00</td>
<td>CENT</td>
</tr>
<tr>
<td>3.53</td>
<td>17.95</td>
<td>MF</td>
</tr>
<tr>
<td>3.42</td>
<td>17.95</td>
<td>GFF</td>
</tr>
<tr>
<td>3.41</td>
<td>17.72</td>
<td>MF</td>
</tr>
<tr>
<td>3.46</td>
<td>17.80</td>
<td>GFF</td>
</tr>
<tr>
<td>3.43</td>
<td>17.80</td>
<td>GFF</td>
</tr>
<tr>
<td>4.22</td>
<td>5.45</td>
<td>MF</td>
</tr>
<tr>
<td>4.23</td>
<td>5.45</td>
<td>GFF</td>
</tr>
<tr>
<td>4.20</td>
<td>5.45</td>
<td>GFF</td>
</tr>
</tbody>
</table>

### Auxiliary Information

Method/Apparatus/Procedure:
- Details given in Gordon and Thorne. Saturated solutions were prepared by equilibrating excess naphthalene and salt solution in an ampoule with shaking for 24 h. The filtered saturated solution was analyzed by a UV spectrophotometer.

Source and Purity of Materials:
- Naphthalene: 99.99 % from James Hinton, Valparaiso, Florida.
- Salts: Analytical reagent grade from Mallinckrodt.
- Natural seawater: Collected at West Falmouth, Buzzards Bay, Quicks Hole, and Mashapaquit Creek, Massachusetts.

Estimated Error:
- Temperature: ±0.03 °C (authors).
- Solubility: ±3 % (authors).

References:
Components: Original Measurements:
(1) Naphthalene: C_{10}H_{8} [91-20-3]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water: H_{2}O; [7732-18-5]

Variables:
One temperature: 24.91 °C
Salinity: 0–108 g/kg sln

Experimental Values
The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[ \log (S) = K_S C_s \]

where

- \( S \) is the solubility (1) in (mg/L);
- \( S \) is the solubility (1) in solution (mg/L);
- \( K_S \) is the Setschenow constant (L/mol);
- \( C_s \) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_s \) 0–2 mol/L, \( K_s = 0.220 \pm 0.0041 \) (95% confidence limit).

The corresponding mass percent and mole fraction, \( x_1 \) at salinity=35 g (2)kg sln calculated by the compilers are 2.36 \( \times 10^{-2} \) g (1/100 g sln and 3.48 \( \times 10^{-4} \) assuming a solution density of 1.025 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
Satrated solutions were prepared by equilibrating excess (1) in salt water in sealed ampoules for 24 h. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.

Source and Purity of Materials:
(1) Recrystallized four times and sublimed or zone refined, 99.99+ % pure.
(2) Analytical reagent grade.
(3) Distilled from potassium permanganate and redistilled from all glass still.

Estimated Error:
Temperature: ±0.03 °C.
Solubility: See above.
Components:
(1) Naphthalene; \( \text{C}_{10}\text{H}_8 \); [91-20-3]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H\(_2\)O; [7732-18-5]

Variables:
One temperature: 25 °C
Salinity: 13–64 g \( \text{kg sln} \)

Experimental Values
Solubility of naphthalene in aqueous sodium chloride at 25 °C

<table>
<thead>
<tr>
<th>( t^\circ\text{C} )</th>
<th>( 10^4 \cdot x_1^a )</th>
<th>( 10^3 \cdot g (1/100 \text{ g sln}) )</th>
<th>( g (2/\text{kg sln})^a )</th>
<th>( g \text{ mol (3/L)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.6</td>
<td>0.84</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11.1</td>
<td>0.92</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14.0</td>
<td>1.09</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17.1</td>
<td>1.23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>1.37</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>23.0</td>
<td>1.58</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25.0</td>
<td>1.73</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>31.8</td>
<td>2.22</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( x_1 \) at 25.0 °C calculated by the compilers are \( 2.17 \cdot 10^{-3} \) g/100 g sln and \( 3.13 \cdot 10^{-6} \).

Auxiliary Information
Method/Apparatus/Procedure:
The solubility of naphthalene in NaCl solution was determined by fluorescence and ultraviolet (UV) absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1×1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostated water bath and then its fluorescent intensity was measured at 350 and 315 nm. The spectrophotometer employed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:
Naphthalene: purity >99 mole %.
Sodium chloride: reagent grade.
Ethanol: reagent grade.
Water: distilled over a KMnO\(_4\)-NaOH solution and passed through a Sephadex column.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±3.3%.
### 2.18. Butlybenzene + Seawater

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Artificial seawater</td>
<td></td>
</tr>
</tbody>
</table>

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Prepared By:**
- M. Kleinschmidt and W. Y. Shiu

**Experimental Values**
The solubility of butylbenzene in artificial seawater is reported to be 7.09 mg (1/100 g sln).

The corresponding mass percent and mole fraction, \( x_1 \), calculated by the compiler, are 7.09 \( \times 10^{-4} \) g (1/100 g sln) and 9.76 \( \times 10^{-4} \), respectively, assuming the artificial seawater composition of Lyman and Fleming. 1

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99% pure.
- (2) Made from doubly distilled water and salts 99% pure.

**References:**

### 2.19. sec-Butlybenzene + Seawater

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Artificial seawater (Lyman and Fleming 1)</td>
<td></td>
</tr>
</tbody>
</table>

**Variables:**
- One temperature: 25.0 °C
- One salinity: 34.5 g salts/kg sln

**Prepared By:**
- M. Kleinschmidt and W. Y. Shiu

**Experimental Values**
The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg (1/100 g sln).

The corresponding mass percent and mole fraction, \( x_1 \), calculated by the compiler are 1.19 \( \times 10^{-3} \) g (1/100 g sln) and 1.64 \( \times 10^{-4} \), respectively, assuming the artificial seawater composition of Lyman and Fleming.1

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99% pure.
- (2) Made from doubly distilled water and salts 99% pure.

**Estimated Error:**
- Temperature: ±0.1 °C.
- Solubility: 0.2 (standard deviation).

**References:**
2.20. tert-Butylbenzene+Seawater

Components:
(1) tert-Butylbenzene; C₇H₁₄; [98-06-6]
(2) Artificial seawater (Ref. 1)

Original Measurements:

Variables:
Prepared By:
One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln
M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of tert-butylbenzene in artificial seawater is reported to be 21.2 mg/kg sln.
The corresponding mass percent and mole fraction \(x_1\), calculated by the compiler, are \(2.12 \times 10^{-3}\) g/100 g sln and \(2.92 \times 10^{-6}\), respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information

Source and Purity of Materials:
(1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 0.3 (standard deviation).

References:

2.21. Decane+Seawater

Components:
(1) Decane; C₁₀H₂₂; [124-18-5]
(2) Seawater

Evaluators:
D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

Critical Evaluation of Solubility of Decane (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Freegarde et al.¹</td>
<td>not specified</td>
<td>not specified</td>
</tr>
<tr>
<td>Krasnoshchekova and Gubergrits²</td>
<td>298</td>
<td>6</td>
</tr>
</tbody>
</table>

Reference solubility data for decane in pure water at 298 K were reported in Part 9, Shaw and Maczynski,³ and converted by the Evaluators to g/100 g sln.
The experimental data are listed in Table 8. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergrits² are considered Doubtful.

Rejected and Inaccessible Data

The data reported by Freegarde et al.¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

Table 8. Experimental values for solubility of decane (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1)/100 g sln (D=doubtful)</th>
<th>Reference value for pure water g (1)/100 g sln ± 50%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 2)</td>
<td>8.7 \times 10^{-6} (D; Ref. 2)</td>
<td>2.6 \times 10^{-6}</td>
</tr>
<tr>
<td>Components:</td>
<td>Original Measurements:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------</td>
<td>------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2) Seawater (composition not specified)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature, pressure, salinity not given</td>
<td>M. Kleinschmidt and D. G. Shaw</td>
</tr>
</tbody>
</table>

**Experimental Values**

The solubility of decane was reported to be 0.15 mg/L. The corresponding mass percent and mole fractions (x<sub>1</sub>), calculated by the compilers, are 1.5 • 10<sup>-5</sup> g (1/100) g sln and 1.9 • 10<sup>-8</sup>, respectively, assuming a solution density of 1.02 kg/L.

**Auxiliary Information**

<table>
<thead>
<tr>
<th>Method/Apparatus/Procedure:</th>
<th>Source and Purity of Materials:</th>
</tr>
</thead>
<tbody>
<tr>
<td>None given except that analysis was done using gas chromatography.</td>
<td>Not given.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Seawater</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>One temperature: 25 °C</td>
<td>M. Kleinschmidt</td>
</tr>
<tr>
<td>Salinity: 6 g/kg sln</td>
<td></td>
</tr>
</tbody>
</table>

**Experimental Values**

The solubility of decane in seawater was reported to be 8.7 • 10<sup>-6</sup> g (1/100) g sln and the corresponding mole fraction, x<sub>1</sub> = 1.1 • 10<sup>-8</sup>.

**Auxiliary Information**

<table>
<thead>
<tr>
<th>Method/Apparatus/Procedure:</th>
<th>Source and Purity of Materials:</th>
</tr>
</thead>
<tbody>
<tr>
<td>A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.</td>
<td>(1) “Chemically pure.”</td>
</tr>
<tr>
<td>(2) Distilled water plus salt mixture.</td>
<td></td>
</tr>
</tbody>
</table>

| Estimated Error: | Not specified. |
### 2.22. 1-Methylnaphthalene + Seawater

**Components:**
1. 1-Methylnaphthalene; C_{11}H_{10}; 90-12-0
2. Sodium chloride; NaCl; 7647-14-5
3. Water; H_{2}O; 7732-18-5

**Variables:**
- Temperature: 8.1–28.5 °C
- Salinity: 30 g (2) kg sln

**Prepared By:**
W. Y. Shiu and D. Mackay

**Experimental Values**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^4 mol/l/L sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.1</td>
<td>1.23</td>
</tr>
<tr>
<td>11.1</td>
<td>1.35</td>
</tr>
<tr>
<td>15.5</td>
<td>1.49</td>
</tr>
<tr>
<td>17.4</td>
<td>1.53</td>
</tr>
<tr>
<td>18.2</td>
<td>1.54</td>
</tr>
<tr>
<td>20.7</td>
<td>1.54</td>
</tr>
<tr>
<td>25.3</td>
<td>1.63</td>
</tr>
<tr>
<td>25.0</td>
<td>1.69</td>
</tr>
<tr>
<td>28.5</td>
<td>1.81</td>
</tr>
</tbody>
</table>

The corresponding mass percent and mole fraction (x_1) at 25.0 °C, calculated by the compiler, are 2.34 \times 10^{-5} g (1)/100 g sln and 3.06 \times 10^{-6}.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The solubility of 1-methylnaphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of 1-methylnaphthalene to an air-tight 1 \times 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least cell 72 h in a thermostated water bath and then its fluorescent intensity was measured at 350 and 320 nm. The spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorbivity of 1-methylnaphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

**Source and Purity of Materials:**
1. 1-Methylnaphthalene: purity >99%.
2. Sodium chloride: reagent grade.
3. Water: distilled over a KMnO_4–NaOH solution and passed through a Sephadex column.

**Estimated Error:**
- Temperature: ±0.1 °C (author).
- Solubility: ±3.0% (author).

### 2.23. Undecane + Seawater

**Components:**
1. Undecane; C_{11}H_{24}; 1120-21-4
2. Seawater

**Variables:**
- One temperature: 25 °C
- Salinity: 6 g/kg sln

**Prepared By:**
M. Kleinschmidt

**Experimental Values**
The solubility of undecane in seawater was reported to be 1.0 \times 10^{-5} g (1)/100 g sln and the corresponding mole fraction, x_1 = 1.2 \times 10^{-9}.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

**Source and Purity of Materials:**
1. “Chemically pure.”
2. Distilled water plus salt mixture.

**Estimated Error:**
Not specified.
2.24. Acenaphthene+Seawater

Components:
(1) Acenaphthene, C12H10; [83-32-9]
(2) Seawater, natural

Original Measurements:

Variables:
Temperature: 15–25 °C
Salinity: 35 g/kg sln

Prepared By:
W. Y. Shiu and D. Mackay

Experimental Values
Solubility of acenaphthene in seawater

<table>
<thead>
<tr>
<th>T/K</th>
<th>10^3 x, g</th>
<th>10^3 g (T/100 g sln)a</th>
<th>µg (T/1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>2.56</td>
<td>2.14</td>
<td>0.214</td>
</tr>
<tr>
<td>20</td>
<td>6.6</td>
<td>5.5</td>
<td>0.55</td>
</tr>
<tr>
<td>25</td>
<td>22.0</td>
<td>18.4</td>
<td>1.84</td>
</tr>
</tbody>
</table>

aCalculated by compilers.

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared by equilibrating seawater with an excess of hydrocarbon for 24 h in a constant temperature gyrotary shaker followed by 12 h stationary period. A 100 mL aliquot was extracted three times with hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the hydrocarbon concentration.

Source and Purity of Materials:
Acenaphthene: from Aldrich Chemical Co. of 99% purity and doubly distilled from distilled methanol.
Hexane: doubly distilled in glass.
Seawater: collected off Scripps Pier and was filtered twice through 0.22 µm membrane and twice extracted with hexane then its salinity adjusted to 35 parts per thousand.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±2%.

2.25. Biphenyl+Seawater

Components:
(1) Biphenyl, C12H10; [92-52-4]
(2) Seawater

Evaluators:
D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

Critical Evaluation of Solubility of Biphenyl (1) in Seawater (2)
The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eganhouse and Calder1</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Paul2</td>
<td>298</td>
<td>13–64</td>
</tr>
</tbody>
</table>

References:

Table 9. Experimental values for solubility of biphenyl (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (T/100 g sln) (T=tentative)</th>
<th>Reference value for pure water g (T/100 g sln) ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>35 (Ref. 1)</td>
<td>4.76·10^{-4} (T; Ref. 1)</td>
<td>7·10^{-4}</td>
</tr>
<tr>
<td>13.25 (Ref. 2)</td>
<td>6.08·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>26.24 (Ref. 2)</td>
<td>5.46·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>39.05 (Ref. 2)</td>
<td>4.62·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>46.28 (Ref. 2)</td>
<td>4.16·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>51.62 (Ref. 2)</td>
<td>4.13·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>63.97 (Ref. 2)</td>
<td>3.54·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>63.97 (Ref. 2)</td>
<td>3.45·10^{-4} (T; Ref. 2)</td>
<td>2.54·10^{-4} (T; Ref. 2)</td>
<td></td>
</tr>
</tbody>
</table>
The solubility of biphenyl in seawater is reported to be 4.76 mg/kg. The corresponding mass percent and mole fraction \(x_1\), calculated by the compilers, are \(4.76 \times 10^{-4}\) g/(100 g sln) and \(5.70 \times 10^{-5}\), respectively. Graphical results for other salinities are also reported.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Equilibrium was obtained in a 50 mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05 °C for at least 48 h, and shaken occasionally during that time. Samples were withdrawn with a 10 mL transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultraviolet region of the spectrum.

**Source and Purity of Materials:**

(1) Recrystallized from methanol.
(2) Reagent grade, dried at 120 °C before weighing.
(3) Redistilled. Sources not specified.

**Estimated Error:**

Temperature: ± 0.05 °C.
Solubility: ± 2.6%.

**References:**

2.26. Dodecane+Seawater

Components: (1) Dodecane; C\textsubscript{12}H\textsubscript{26}; [112-40-3] (2) Seawater

Components: Original Measurements:
(1) Dodecane; C\textsubscript{12}H\textsubscript{26}; [112-40-3] (2) Salt mixture (Ref. 1) (2) Water; H\textsubscript{2}O; [7732-18-5]

Components: Evaluators:
D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

Critical Evaluation of Solubility of Dodecane (1) in Seawater (2)
The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Reference solubility data for dodecane in pure water at 298 K were reported in Part 10, Shaw and Maczynski, and converted by the Evaluators to g/100 g sln.

The experimental data are listed in Table 10. The reported data are all from different salinities, which precludes direct comparison. The data are in only fair agreement with each other and with the reference values for the solubility of dodecane in pure water. Since hydrocarbon solubilities in saline solutions are expected to be less than in pure water, the data of Krasnoshchekova and Gubergrits are Doubtful. The remaining data are Tentative.

References:

Experimental Values
Dodecane concentration in saline medium after gently stirring for 1 week and then remaining quiescent for the periods shown.

<table>
<thead>
<tr>
<th>Time (weeks)</th>
<th>Dodecene, µg (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.16±0.03</td>
</tr>
<tr>
<td>8</td>
<td>1.80±0.02</td>
</tr>
<tr>
<td>16</td>
<td>1.78±0.02</td>
</tr>
</tbody>
</table>

The corresponding mass percent and mole fraction calculated by the compilers for the results at 16 weeks is 1.74 \( \cdot 10^{-7} \) g (1/100 g sln) and 1.89 \( \cdot 10^{-10} \) using the assumption that the solution density is 1.02 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
Dodecane solutions were prepared in a chemically defined solution resembling dilute seawater. In addition to the mineral salts and vitamins reported (Button), the solution contained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121 °C for 30 min), 0.8 µL of \(^{13}C\)-dodecane was sprayed on to the medium surface to form a thin film. Gentle subsurface agitation was induced by a 3 in. magnet rotating at 60 rpm against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples collected from a port at the bottom of the carboy. The system was stirred for 1 week and then allowed to stand. Equilibrium appeared to have been achieved within 8 weeks.

Source and Purity of Materials:
Amersham Searle Corp. (Arlington Heights, IL) supplied the \([1-^{13}C]\) dodecane, 27 µCi/µmol. It was accompanied by a gas chromatogram of the preparation showing a single peak at the appropriate location.

Estimated Error:
Experimental error is estimated at ±1%.

References:

Table 10. Experimental values for solubility of dodecane (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln) T=tentative, D=Doubtful</th>
<th>Reference value for pure water g (1/100 g sln) ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>12 (Ref. 1)</td>
<td>1.74 ( \cdot 10^{-7} ) (T; Ref. 1)</td>
<td>3.4 ( \cdot 10^{-7} )</td>
</tr>
<tr>
<td></td>
<td>6 (Ref. 2)</td>
<td>5 ( \cdot 10^{-7} ) (D; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>35 (Ref. 3)</td>
<td>2.9 ( \cdot 10^{-7} ) (T; Ref. 3)</td>
<td></td>
</tr>
</tbody>
</table>
**Components:**
(1) Dodecane; C12H26 \( [112-40-3] \)
(2) Seawater

**Variables:**
One temperature: 25 °C
Salinity: 6 g/kg sln

**Prepared By:**
M. Kleinschmidt

**Experimental Values**
The solubility of dodecane in seawater was reported to be 5 \( \times \) 10\(^{-7}\) g \( (1/100 \text{ g sln} \) and the corresponding mole fraction \( x_1 = 5.0 \times 10^{-10} \).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

**Source and Purity of Materials:**
(1) “Chemically pure.”
(2) Distilled water plus salt mixture.

**Estimated Error:**
Not specified.

---

**Components:**
(1) Dodecane; C12H26 \( [112-40-3] \)
(2) Seawater

**Variables:**
One temperature: 25 °C
One salinity: 35 g salts/kg sln

**Prepared By:**
P. A. Meyers and D. G. Shaw

**Experimental Values**
The solubility of dodecane in seawater was reported to be 2.9 \( \times \) 10\(^{-7}\) g \( (1/100 \text{ g sln} \) and \( x_1 = 3.1 \times 10^{-10} \).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0±0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 \( \mu \text{m} \) membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
Analabs, Inc., North Haven, Conn. 99+ % pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with \( \text{HgCl}_2 \) sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural \( n \)-alkane levels too low to cause interference.

**Estimated Error:**
Eight replications were made. The average of the deviations of the mean gave an experimental error of \( \pm 16\% \), yet some accommodation may have occurred due to presence of natural dissolved organic matter.
### 2.27. Fluorene-Seawater

**Components:**
- (1) Fluorene; C13H10; [86-73-7]
- (2) Sodium chloride; NaCl; [7647-14-5]
- (3) Water; H2O; [7732-18-5]

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 0–40 g salts/kg sln

**Prepared By:**
- W. Y. Shiu and D. Mackay

**Experimental Values**

The solubility of fluorene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[ \log(S/0.15) = K_S C_s \]

where
- \( S \) is the solubility of (1) in solution (mg/L);
- \( S_0 \) is the solubility of (1) in water (mg/L);
- \( K_S \) is the Setschenow constant (L/mol);
- \( C_s \) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_s \) 0–0.7 mol/L, \( K_S = 0.267 \) with \( S_0 = 1.685 \).

The corresponding mass percent and mole fraction, \( x \), at salinity 0.5 g/100 g sln calculated by the compilers are 1.20 \( \times 10^{-4} \) g/100 g sln and 1.30 \( \times 10^{-3} \).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
- A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C18 stationary phase. Then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

**Source and Purity of Materials:**
- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

**Estimated Error:**
- Temperature: ±0.05 °C.

### 2.28. Anthracene-Seawater

**Components:**
- (1) Anthracene; C14H10; [120-12-7]
- (2) Seawater

**Evaluators:**
- D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

**Critical Evaluation of Solubility of Anthracene (1) in Seawater (2)**

The experimental solubility data for (1) in (2) have been investigated by the authors listed below.

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>May et al.1</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Schwarz2</td>
<td>281–303</td>
<td>30</td>
</tr>
</tbody>
</table>

Mean of selected experimental solubility data for anthracene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,3 and converted by the Evaluators to g (1/100 g sln).

The experimental data are listed in Table 11. The reported data are from different salinities, which precludes direct comparison. Since the data appear consistent with each other and with the mean value for the solubility of anthracene in pure water, the data of May et al.1 and Schwarz2 are adopted as Tentative. Schwarz2 also reports data over the temperature range.

**References:**

#### Table 11. Experimental values for solubility of anthracene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1/100 g sln) (T=tentative)</th>
<th>Mean value for pure water g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>35 (Ref. 1)</td>
<td>3.11 ( \times 10^{-6} ) (T; Ref. 1)</td>
<td>4.3 ( \times 10^{-6} )</td>
</tr>
<tr>
<td>30</td>
<td>30 (Ref. 2)</td>
<td>3.55 ( \times 10^{-6} ) (T; Ref. 2)</td>
<td></td>
</tr>
</tbody>
</table>
Components:
(1) Anthracene; C_{14}H_{10}; [120-12-7]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_{2}O; [7732-18-5]

Variables:
One temperature: 25 °C
Salinity: 0–40 g (2)kg sln

Experimtal Values

The solubility of anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[
\log(S_{0}/S) = K_{S}C_s
\]

where

- \( S_{0} \) is the solubility of (1) in water (mg/L);
- \( S \) is the solubility of (1) in solution (mg/L);
- \( K_{S} \) is the Setschenow constant (L/mol); and
- \( C_s \) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_s \), \( 0.238 \) with \( S_{0} = 0.0446 \).

The corresponding mass percent and mole fraction \( x_{1} \) at salinity=35 g (2)kg sln, calculated by the compilers, are \( 3.11 \times 10^{-6} \) g (1/100 g sln and \( 3.22 \times 10^{-6} \).

Source and Purity of Materials:
(1) Greater than 97% pure.
(2) Reagent grade.
(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:
Temperature: \( \pm 0.05^\circ\text{C} \)
\( K_{S} \): \( \pm 0.004 \)
\( S_{0} \): \( \pm 0.0002 \)

Separate methods of analysis used for the solubility were determined in NaCl solution was prepared by adding excess amount of anthracene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 ml of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 365 nm. The spectrophotometer employed a ratio-photon counting mode where anthracene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorbivity of anthracene in ethanol solution therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:
(1) Anthracene; purity \( >99 \) mole %.
Sodium chloride: reagent grade.
Water: distilled over a KMnO_{4}-NaOH solution and passed through a Sephadex column.
Ethanol: reagent grade.

Estimated Error:
Temperature: \( \pm 0.1^\circ\text{C} \) (author).
Solubility: \( \pm 4.3\% \) (author).
2.29. Phenanthrene+Seawater

Components:
(1) Phenanthrene; C14H10; [85-01-8]
(2) Seawater

Evaluators:
D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

Critical Evaluation of Solubility of Phenanthrene (1) in Seawater (2)
The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salt/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquan-Yuen et al.¹</td>
<td>298</td>
<td>29–108</td>
</tr>
<tr>
<td>Eganhouse and Calder²</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>May et al.³</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Schwarz⁴</td>
<td>284–305</td>
<td>30</td>
</tr>
</tbody>
</table>

Mean of selected experimental solubility data for phenanthrene in pure water at 298 K was reported in Part 11, Shaw and Maczynski,⁵ and converted by the Evaluators to g (1/100 g sln).

The experimental data are listed in Table 12. At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder² and of May et al.³ are in very good agreement. Therefore their mean, 6.9 × 10⁻² g (1/100 g sln), is adopted as the Recommended value for the solubility of phenanthrene at the indicated temperature and salinity. The value of Aquan-Yuen et al.¹ appears consistent with the data discussed above and with the mean value for the solubility of phenanthrene in pure water and is Tentative. The value of Schwarz⁴ appears slightly high and is considered Doubtful. Schwarz⁴ also reports data over a temperature range.

References:

**Experimental Values**

Solubility of phenanthrene in aqueous NaCl

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salt/kg sln</th>
<th>Experimental values g (1/100 g sln)</th>
<th>Mean value g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>35</td>
<td>6.9 × 10⁻⁵ (R; mean from Refs. 2 and 3)</td>
<td>1.2 × 10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>28.6 (Ref. 1)</td>
<td>8.3 × 10⁻⁵ (T; Ref. 1)</td>
<td>8.3 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>56.2 (Ref. 1)</td>
<td>6.4 × 10⁻⁵ (T; Ref. 1)</td>
<td>6.4 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>82.6 (Ref. 1)</td>
<td>4.5 × 10⁻⁵ (T; Ref. 1)</td>
<td>4.5 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>108.2 (Ref. 1)</td>
<td>3.1 × 10⁻⁵ (T; Ref. 1)</td>
<td>3.1 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>35 (Ref. 2)</td>
<td>7.1 × 10⁻⁵ (R; Ref. 2)</td>
<td>7.1 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>35 (Ref. 3)</td>
<td>6.63 × 10⁻⁵ (R; Ref. 3)</td>
<td>6.63 × 10⁻⁵</td>
</tr>
<tr>
<td></td>
<td>30 (Ref. 4)</td>
<td>9.94 × 10⁻⁵ (D; Ref. 4)</td>
<td>9.94 × 10⁻⁵</td>
</tr>
</tbody>
</table>

ÈCalculated by compilers using density and other physical data for NaCl solutions from Weast.¹

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 h and then allowed to settle for 48 h. An aliquot was extracted with cyclohexane which was then analyzed spectrophotometrically.

Source and Purity of Materials:
(1) Fluorescence grade: from Eastman Kodak.
(2) Reagent grade: from Fisher Scientific.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: ±3 relative %.

References:
Components:  
(1) Phenanthrene; C₁₄H₁₀; [85-01-8]  
(2) Artificial seawater (Lyman and Fleming)  

Variables:  
One temperature 25 °C  
Salinity: 35 g/kg sln

Experimental Values
The solubility of phenanthrene in seawater is reported to be 0.71 mg/kg sln. The corresponding mass percent and mole fraction \(x₁\), calculated by the compilers, are \(7.1 \times 10^{-5}\) g/100 g sln and \(7.4 \times 10^{-8}\), respectively. Graphical results for other salinities are also reported.

Auxiliary Information
Method/Apparatus/Procedure:
Equilibrium was obtained in an Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated at 25 °C for 24 h stationary equilibrium period followed. Hydrocarbons were extracted with twice distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard. Analysis was by gas chromatography.

Source and Purity of Materials:
Analytical grade salt for artificial seawater solution: reagent grade. Water: doubly distilled.

Estimated Error:
Temperature: ±0.5 °C. Solubility: ±0.025 (95% confidence interval).

References:

Components:  
(1) Phenanthrene; C₁₄H₁₀; [85-01-8]  
(2) Sodium chloride; NaCl; [7647-14-5]  
(3) Water; H₂O; [7732-18-5]

Variables:  
One temperature 25 °C  
Salinity: 0–40 g/kg sln

Experimental Values
The solubility of phenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[
\log\frac{S}{S₀} = K_S C_S
\]

where \(S₀\) is the solubility of (1) in water (mg/L); \(S\) is the solubility of (1) in solution (mg/L); \(K_S\) is the Setschenow constant (L/mol); and \(C_S\) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \(S\) over the range of \(C_S 0.0–0.7\) mol/L, \(K_S = 0.275\) with \(S₀ = 1.002\).

The corresponding mass percent and mole fraction \(x₁\) at salinity 35 g (20/kg sln, calculated by the compilers, are \(6.63 \times 10^{-5}\) g/100 g sln and \(6.78 \times 10^{-8}\), respectively. Graphical data for other temperatures are also reported.

Auxiliary Information
Method/Apparatus/Procedure:
A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C₁₈ stationary phase. Then the water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:
(1) Greater than 97% pure.  
(2) Reagent grade.  
(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:
Temperature: ±0.05 °C. \(K_S\): ±0.010. \(S₀\): ±0.011.
Table 1: Solubility of Phenanthrene in NaCl Solution

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (g/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.1</td>
<td>2.88</td>
</tr>
<tr>
<td>14.0</td>
<td>3.2</td>
</tr>
<tr>
<td>17.5</td>
<td>4.07</td>
</tr>
<tr>
<td>20.2</td>
<td>4.51</td>
</tr>
<tr>
<td>23.2</td>
<td>5.75</td>
</tr>
<tr>
<td>25.0</td>
<td>5.72</td>
</tr>
<tr>
<td>29.3</td>
<td>7.2</td>
</tr>
<tr>
<td>31.8</td>
<td>7.9</td>
</tr>
</tbody>
</table>

The corresponding mass percent and mole fraction (x) at 25.0 °C, calculated by the compilers, are 9.94 × 10⁻³ g (1/100 g sln and 1.034 × 10⁻¹, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of phenanthrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of phenanthrene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 ml of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 365 nm. The spectrophotometer employed a ratio–photon counting mode where phenanthrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:
(1) Phenanthrene: purity 99.9%.
(2) Sodium chloride: reagent grade.
(3) Water: distilled over a KMnO₄–NaOH solution and passed through a Sephadex column.
(4) Ethanol: reagent grade.

Estimated Error:
Temperature: ±0.1 °C (author).
Solubility: ±8.4% (author).

Table 2: Solubility of Tetradecane in Seawater

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (g/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.7 × 10⁻⁷</td>
</tr>
</tbody>
</table>

The corresponding mass percent and mole fraction (x) at 25.0 °C, calculated by the compilers, are 1.5 × 10⁻¹0.5 g (1/100 g sln and 1.034 × 10⁻¹, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of tetradecane in seawater was reported to be 1.7 × 10⁻⁷ g (1/100 g sln and x = 1.5 × 10⁻¹⁰.

Source and Purity of Materials:
(1) Tetradecane: purity 99.9%.
(2) Seawater

Estimated Error:
Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.
### 2.31. 2-Methylanthracene + Seawater

**Components:**
- 2-Methylanthracene; C_{15}H_{12} (7647-14-5)
- Sodium chloride; NaCl (7732-18-5)
- Water; H_{2}O (7732-18-5)

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 0–40 g/kg sln

**Experimental Values**

The solubility of 2-methylanthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[ \log(S/S_0) = K_a C_s \]

where:
- \( S_0 \) is the solubility of (1) in water (mg/L);
- \( S \) is the solubility of (1) in solution (mg/L);
- \( K_a \) is the Setschenow constant (L/mol); and
- \( C_s \) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_s \) 0–0.7 mol/L, \( K_a \) = 0.336 with \( S_0 \) = 0.0213.

The corresponding mass percent and mole fraction (\( x_1 \)) at salinity=35 g (2)kg sln, calculated by the compilers, are \( 1.29 \times 10^{-5} \) g (1/100 g sln and \( 1.24 \times 10^{-3} \), respectively.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (3). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

**Source and Purity of Materials:**
- Greater than 97% pure.
- Reagent grade.
- Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

**Estimated Error:**
- Temperature: ±0.05 °C.
- \( K_a \): ±0.006.
- \( S_0 \): ±0.003.

### 2.32. 1-Methylphenanthrene + Seawater

**Components:**
- 1-Methylphenanthrene; C_{15}H_{12} (832-69-9)
- Sodium chloride; NaCl (7647-14-5)
- Water; H_{2}O (7732-18-5)

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 0–40 g/kg sln

**Experimental Values**

The solubility of 1-methylphenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[ \log(S/S_0) = K_a C_s \]

where:
- \( S_0 \) is the solubility of (1) in water (mg/L);
- \( S \) is the solubility of (1) in solution (mg/L);
- \( K_a \) is the Setschenow constant (L/mol); and
- \( C_s \) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_s \) 0–0.7 mol/L, \( K_a \) = 0.211 with \( S_0 \) = 0.269.

The corresponding mass percent and mole fraction (\( x_1 \)) at salinity=35 g (2)kg sln, calculated by the compilers, are \( 1.95 \times 10^{-5} \) g (1/100 g sln and \( 1.87 \times 10^{-3} \), respectively.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (3). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

**Source and Purity of Materials:**
- Greater than 97% pure.
- Reagent grade.
- Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

**Estimated Error:**
- Temperature: ±0.05 °C.
- \( K_a \): ±0.018.
- \( S_0 \): ±0.003.
2.33. Fluoranthene+Seawater

Components:
(1) Fluoranthene; C16H10; [206-44-0]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H2O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C
Salinity: 0–40 g (2)/kg sln

Experimental Values
The solubility of fluoranthene in aqueous sodium chloride is reported in terms of the Setschenow equation:
\[ \log(S_0/S) = K_S C_S \]

where
- \( S_0 \): the solubility of (1) in water (mg/L);
- \( S \): the solubility of (1) in solution (mg/L);
- \( K_S \): the Setschenow constant (L/mol);
- \( C_S \): the concentration of sodium chloride (L/mol).

When evaluating the equation for \( S \) over the range of \( C_S \), 0–0.7 mol/L, \( K_S = 0.399 \) with \( S_0 = 0.206 \).

The corresponding mass percent and mole fraction (\( x_1 \)) at salinity=35 g (2)/kg sln, calculated by the compilers, are 1.24 \( \times 10^{-3} \) g (1)/100 g sln and 1.14 \( \times 10^{-3} \), respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C8 stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:
(1) Greater than 97% pure.
(2) Reagent grade.
(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:
Temperature: ± 0.05 °C.
\( K_S \): ± 0.010.
\( S_0 \): ± 0.002.

2.34. Pyrene+Seawater

Components:
(1) Pyrene; C16H10; [129-00-0]
(2) Seawater

Critical Evaluation of Solubility of Pyrene (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Krasnoshchekova et al.1</td>
<td>298</td>
<td>6</td>
</tr>
<tr>
<td>May et al.2</td>
<td>298</td>
<td>35</td>
</tr>
<tr>
<td>Rossi and Thomas3</td>
<td>288–298</td>
<td>35</td>
</tr>
<tr>
<td>Schwarz4</td>
<td>282–304</td>
<td>30</td>
</tr>
</tbody>
</table>

Mean of selected experimental solubility data for pyrene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,5 and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 13. At 298 K and a salinity of 35 g salts/kg sln, calculated by the compilers, are 1.24 \( \times 10^{-3} \) g (1)/100 g sln and 1.14 \( \times 10^{-3} \).

The corresponding mass percent and mole fraction (\( x_1 \)) at salinity=35 g (2)/kg sln, calculated by the compilers, are 1.24 \( \times 10^{-3} \) g (1)/100 g sln and 1.14 \( \times 10^{-3} \), respectively.

References:

Table 13. Experimental values for solubility of pyrene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1)/100 g sln</th>
<th>Mean value for pure water g (1)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 1)</td>
<td>7.705 ( \times 10^{-6} ) (R; Ref. 1)</td>
<td>1.4 ( \times 10^{-5} )</td>
</tr>
<tr>
<td>35</td>
<td>35 (Ref. 2)</td>
<td>8.6 ( \times 10^{-6} ) (R; Ref. 2)</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>35 (Ref. 3)</td>
<td>8.9 ( \times 10^{-6} ) (T; Ref. 3)</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>30 (Ref. 4)</td>
<td>9.48 ( \times 10^{-6} ) (T; Ref. 4)</td>
<td></td>
</tr>
</tbody>
</table>
Components: 
(1) Pyrene; C_{16}H_{10}; [129-00-0] 
(2) Salt water 

Variables: 
One temperature: 25 °C 
Salinity: 6 g/kg sln 

Prepared By: 
M. Kleinschmidt and D. G. Shaw 

Experimental Values 
The solubility of pyrene in salt water was reported to be 78.9 μg/L. 
The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 7.705 × 10^{-6} • 100 g sln and 7.02 × 10^{-6}, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information 
Method/Apparatus/Procedure: 
A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C_{18} stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials: 
(1) Greater than 97% pure. 
(2) Reagent grade. 
(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column. 

Estimated Error: 
Temperature: ± 0.05 °C. 
K_2: ± 0.003. 
S_2: ± 0.001.
Components: Original Measurements:
(1) Pyrene: C_{16}H_{10} [129-00-0]
(2) Seawater; natural


Variables:
Temperature: 15–25 °C
Salinity: 35 g/kg sln

Prepared By:
W. Y. Shiu and D. Mackay

Experimental Values
Solubility of pyrene in seawater

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^7 x_i^2</th>
<th>10^6 g (1/100 g sln)</th>
<th>µg (1/100 g) (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>5.1</td>
<td>5.6</td>
<td>0.056</td>
</tr>
<tr>
<td>20</td>
<td>6.5</td>
<td>7.1</td>
<td>0.071</td>
</tr>
<tr>
<td>25</td>
<td>8.1</td>
<td>8.9</td>
<td>0.089</td>
</tr>
</tbody>
</table>

*Calculated by compilers.

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solution was prepared by equilibrating seawater with an excess of pyrene for at least 24 h in a constant-temperature gyrotary shaker followed by a 12 h stationary equilibration period. A 100 mL aliquot was extracted three times with n-hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the pyrene concentration.

Source and Purity of Materials:
Pyrene: from Aldrich Chemical Co. and purified with 2,4,6-trinitrophenol.
n-Hexane: doubly distilled in glass.
Seawater: collected off Scripps Pier and was filtered twice through 0.22 μm membrane and twice extracted with n-hexane then its salinity was adjusted to 35%.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±11%.

Components: Original Measurements:
(1) Pyrene: C_{16}H_{10} [129-00-0]
(2) Sodium chloride; NaCl [7647-14-5]
(3) Water; H2O [7732-18-5]


Variables:
Temperature: 8.6–31.1 °C
Salinity: 30 g (2/100 g sln)

Prepared By:
W. Y. Shiu and D. Mackay

Experimental Values
Solubility of pyrene in 0.5 g mol (2/10 L sln

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^2 mol (1/10 L sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.6</td>
<td>2.00</td>
</tr>
<tr>
<td>12.2</td>
<td>2.50</td>
</tr>
<tr>
<td>15.5</td>
<td>2.85</td>
</tr>
<tr>
<td>18.2</td>
<td>3.22</td>
</tr>
<tr>
<td>20.7</td>
<td>3.57</td>
</tr>
<tr>
<td>23.0</td>
<td>3.90</td>
</tr>
<tr>
<td>25.0</td>
<td>4.41</td>
</tr>
<tr>
<td>28.1</td>
<td>5.19</td>
</tr>
<tr>
<td>31.1</td>
<td>5.96</td>
</tr>
</tbody>
</table>

The corresponding mass percent and mole fraction (x_i) at 25.0 °C, calculated by the compilers, are 9.48 · 10^6 g (1/100 g sln and 7.97 · 10^-5, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostated water bath and then its fluorescence intensity was measured at 365 nm. The spectrofluorimeter employed a ratio-photon counting mode where pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of pyrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:
(1) Pyrene: purity >99 mole %.
Sodium chloride: reagent grade.
Water: distilled over a KMnO_4-NaOH solution and passed through a Sephadex column.
Ethanol: reagent grade.

Estimated Error:
Temperature: ±0.1 °C (author).
Solubility: ±1.6% (author).
### 2.35. Hexadecane+Seawater

**Components:**
- (1) Hexadecane, C\textsubscript{16}H\textsubscript{34}; [544-76-3]
- (2) Seawater

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- One salinity: 35 g salts/kg sln

**Prepared By:**
- P. A. Meyers and D. G. Shaw

**Experimental Values**

The solubility of hexadecane in seawater was reported to be 4 × 10\textsuperscript{-8} g/100 g sln and x\textsubscript{1} = 3 × 10\textsuperscript{-11}.  

**Auxiliary Information**

**Method/Apparatus/Procedure:**
- (1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- Analabs, Inc., North Haven, Conn. 99% pure hydrocarbons.
- Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl\textsubscript{2} sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

**Estimated Error:**
- Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accomodation may have occurred due to presence of natural dissolved organic matter.

### 2.36. Benz[a]anthracene+Seawater

**Components:**
- (1) Benz[a]anthracene, C\textsubscript{18}H\textsubscript{12}; [56-55-3]
- (2) Seawater

**Prepared By:**
- D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.

**Critical Evaluation of Solubility of Benz[a]anthracene (1) in Seawater (2)**

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

**Author(s)**
- Krasnosnchekova et al.\textsuperscript{1}
- May et al.\textsuperscript{2}

**T/K**
- 298

**Salinity g salts/kg sln**
- 6
- 35

Mean of selected experimental solubility data for benz[a]anthracene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,\textsuperscript{3} and converted by the Evaluators to g (1/100) g sln.

The experimental data are listed in Table 14. The value reported by May et al.\textsuperscript{2} was derived from several measurements using the Setschenow equation and is consistent with the mean value for the solubility of benz[a]anthracene in pure water. Therefore their value is adopted as Tentative. The value of Krasnosnchekova et al.\textsuperscript{1} appears slightly low and is considered Doubtful.  

**References:**

**Table 14. Experimental values for solubility of benz[a]anthracene (1) in seawater (2)**

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values g (1/100 g sln)</th>
<th>Mean value for pure water g (1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 1) 6.2 × 10\textsuperscript{-8} (D, Ref. 1)</td>
<td>9.2 × 10\textsuperscript{-7}</td>
</tr>
<tr>
<td>35</td>
<td>5.6 × 10\textsuperscript{-7} (T, Ref. 2)</td>
<td></td>
</tr>
</tbody>
</table>
Components: Original Measurements:
(1) Benz[a]anthracene; C_{18}H_{12}·[56-55-3]
(2) Salt water


Variables: Prepared By:
One temperature: 25 °C
Salinity: 6 g/kg sln

M. Kleinschmidt and D. G. Shaw

Experimental Values
The solubility of benz[a]anthracene in salt water was reported to be 0.63 g/L.
The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 6.2 \times 10^{-3} g/100 g sln and 5.2 \times 10^{-11}, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:
Not given.

Estimated Error:
Temperature: ±1 °C
Solubility: ±0.075, type of error not specified.

References:

Components: Original Measurements:
(1) Benz[a]anthracene; C_{18}H_{12}·[56-55-3]
(2) Sodium chloride; NaCl [7647-14-5]
(3) Water; H_{2}O [7732-18-5]


Variables: Prepared By:
One temperature: 25 °C
Salinity: 0–40 g/kg sln

W. Y. Shiu and D. Mackay

Experimental Values
The solubility of benz[a]anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[
\log S_1/S_0 = KS_C
\]

where:
- \(S_0\) is the solubility of (1) in water (mg/L);
- \(S\) is the solubility of (1) in solution (mg/L);
- \(K_S\) is the Setschenow constant (L/mole); and
- \(C\) is the concentration of sodium chloride (L/mole).

When evaluating the equation for \(S\) over the range of \(C\) 0–0.7 mol/L, \(K_S\) = 0.354 with \(S_0\) = 0.0094.
The corresponding mass percent and mole fraction (x_1) at salinity=35 g (20 kg sln, calculated by the compilers, are 5.6 \times 10^{-3} g/100 g sln and 4.5 \times 10^{-10}, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:
(1) Greater than 97% pure.
(2) Reagent grade.
(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:
Temperature: ±0.05 °C.
\(K_S\) = ±0.002.
\(S_0\) = ±0.001.
### 2.37. Chrysene + Seawater

**Components:**
1. Chrysene: C18H12; [218-01-9]
2. Sodium chloride: NaCl; [7647-14-5]

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 0–40 g salts/kg sln

**Prepared By:**
W. Y. Shiu and D. Mackay

**Experimental Values**

The solubility of chrysene in aqueous sodium chloride is reported in terms of the Setschenow equation:

\[
\log \left( \frac{S}{S_0} \right) = K_S C_S
\]

where
- \(S_0\) is the solubility of chrysene in water (mg/L);
- \(S\) is the solubility of chrysene in solution (mg/L);
- \(K_S\) is the Setschenow constant (L/mol); and
- \(C_S\) is the concentration of sodium chloride (L/mol).

When evaluating the equation for \(S\) over the range of \(C_S\) 0–0.7 mol/L, \(K_S = 0.336, S_0 = 0.0018\).

The corresponding mass percent and mole fraction \(x_1\) at salinity 35 g salts/kg sln, calculated by the compilers, are \(1.1 \times 10^{-7} \text{ g (1L/100 g sln)}\) and \(8.8 \times 10^{-11}\), respectively.

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution of chrysene was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of chrysene. The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C18 stationary phase. A water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of chrysene was measured with a UV detector.

**Source and Purity of Materials:**
- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

**Estimated Error:**
Temperature: ±0.05 °C
\(K_S: \pm 0.010\)
\(S_0: \pm 0.0001\)

### 2.38. Octadecane + Seawater

**Components:**
1. Octadecane: C18H38; [593-45-3]
2. Seawater

**Original Measurements:**

**Variables:**
- One temperature: 25 °C
- Salinity: 35 g salts/kg sln

**Prepared By:**
P. A. Meyers and D. G. Shaw

**Experimental Values**

The solubility of octadecane in seawater was reported to be \(8 \times 10^{-8} \text{ g (1L/100 g sln)}\) and \(x_1 = 5 \times 10^{-11}\).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A saturated solution of octadecane and seawater was placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

**Source and Purity of Materials:**
- (1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.
- Analabs, Inc., North Haven, Conn. 99% pure hydrocarbons.
- Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl2 sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

**Estimated Error:**
Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.
2.39. Benzo[a]pyrene+Seawater

Components:
1. Benzo[a]pyrene; C20H12; [50-32-8]
2. Salt water

Original Measurements:

Variables:
One temperature: 25 °C
Salinity: 6 g/kg sln (Ref. 1)

Prepared By:
M. Kleinschmidt and D. G. Shaw

The solubility of benzo[a]pyrene in salt water was reported to be 0.13 g/L. The corresponding mass percent and mole fraction \(x_1\), calculated by the compilers, are \(1.3 \times 10^{-8}\ g/100\ g\ sln\) and \(9.5 \times 10^{-12}\), respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 \(g\) to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasi-linear luminescence spectra.

Source and Purity of Materials:
Not given.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.008; Type of error not specified.

References:

Critical Evaluation of Solubility of Benzo[e]Pyrene (1) in Seawater (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>Krasnoschekova et al.</td>
<td>298</td>
<td>6</td>
</tr>
<tr>
<td>Schwarz2</td>
<td>298</td>
<td>30</td>
</tr>
</tbody>
</table>

The experimental data are listed in Table 15. The two reported values are in fair agreement and therefore both are adopted as Tentative at their respective salinities. Schwarz also provides data over the temperature range 282–303 K.

References:

Table 15. Experimental values for solubility of benzo[e]pyrene (1) in seawater (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Salinity g salts/kg sln</th>
<th>Experimental values g (1)/100 g sln ((T)=tentative)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>6 (Ref. 1)</td>
<td>1.79 \times 10^{-7} (T; Ref. 1)</td>
</tr>
<tr>
<td>30</td>
<td>(Ref. 2)</td>
<td>3.32 \times 10^{-7} (T; Ref. 2)</td>
</tr>
</tbody>
</table>
Components: (1) Benzo[e]pyrene; C_{20}H_{12}; [192-97-2] (2) Salt water

Variables: Prepared By:
One temperature: 25 °C
Salinity: 6 g/kg sln

Prepared By: M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benzo[e]pyrene in salt water was reported to be 1.83 g/L.
The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 1.79 \times 10^{-7} g/100 g sln and 1.34 \times 10^{-10}, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of benzo[e]pyrene to an air-tight 1 \times 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 410 and 265 nm. The spectrofluorimeter employed a ratio-photon counting mode where benzo[e]pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore providing an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:
(1) Benzo[e]pyrene: purity >99 mole %.
Sodium chloride: reagent grade.
Water: distilled over a KMnO_4-NaOH solution and passed through a Sephadex column.
Cyclohexane: reagent grade.

Estimated Error:
Temperature: ±0.1 °C (author).
Solubility: ±19.5% (author).
2.41. Eicosane + Seawater

Components:
(1) Eicosane, C\textsubscript{20}H\textsubscript{42}; [112-95-8]
(2) Seawater

Original Measurements:

Variables:
One temperature: 25 °C
Salinity: 35 g salts/kg sln

Experimental Values
The solubility of eicosane in seawater was reported to be $8 \times 10^{-8}$ g (1/100 g sln and $x_1 = 5 \times 10^{-11}$.

Auxiliary Information

Method/Apparatus/Procedure:
One temperature: 25 °C
Salinity: 35 g salts/kg sln

Source and Purity of Materials:
Analabs, Inc., North Haven, Conn. 99% pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl\textsubscript{2} sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural \(n\)-alkane levels too low to cause interference.

Estimated Error:
Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.42. Benzo[ghi]perylene + Seawater

Components:
(1) Benzo[ghi]perylene, C\textsubscript{22}H\textsubscript{12}; [191-24-2]
(2) Salt water

Original Measurements:

Variables:
One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits)

Experimental Values
The solubility of benzo[ghi]perylene in salt water was reported to be 0.21 g/L. The corresponding mass percent and mole fraction \((x_1)\), calculated by the compilers, are $2.1 \times 10^{-8}$ g (1/100 g sln and $1.4 \times 10^{-11}$ assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

References:
2.43. Benzo[b]triphenylene + Seawater

Components: (1) Benzo[b]triphenylene; C_{22}H_{14}; [215-58-7] (2) Salt water


Variables: One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits)

Prepared By: M. Kleinschmidt and D. G. Shaw

Experimental Values
The solubility of benzo[b]triphenylene in salt water was reported to be 27.84 g/L.
The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 2.719 x 10^{-6} g/100 g sln and 1.841 x 10^{-9}, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L of water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials: Not given.

Estimated Error:
Temperature: ± 1 °C
Solubility: ± 1.48; type of error not specified.

References:

2.44. Dibenz[a,h]anthracene + Seawater

Components: (1) Diben[a,h]anthracene; C_{22}H_{14}; [53-70-3] (2) Salt water


Variables: One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits)

Prepared By: M. Kleinschmidt and D. G. Shaw

Experimental Values
The solubility of diben[a,h]anthracene in salt water was reported to be 21.13 g/L.
The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 2.064 x 10^{-6} g/100 g sln and 1.397 x 10^{-9}, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information

Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L of water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials: Not given.

Estimated Error:
Temperature: ± 1 °C
Solubility: ± 1.14; type of error not specified.

References:
**2.45. Dibenzo[a]anthracene + Seawater**

**Components:**
(1) Dibenzo[a]anthracene; C_{22}H_{14} 
(2) Salt water

**Original Measurements:**

**Variables:**
One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits)

**Prepared By:**
M. Kleinschmidt and D. G. Shaw

Experimental Values
The solubility of dibenz[a]anthracene in salt water was reported to be 10.544 g/L. The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are 1.029 \times 10^{-6} \text{g/100 g sln} and 6.970 \times 10^{-12}, respectively, assuming a solution density of 1.004 kg/L.

**Auxiliary Information**
Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating; 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:
Not given.

**Estimated Error:**
Temperature: \pm 1 °C
Solubility: \pm 1.05; type of error not specified.

**References:**

**2.46. Hexacosane + Seawater**

**Components:**
(1) Hexacosane; C_{26}H_{54} ; [630-01-3]
(2) Seawater

**Original Measurements:**
P. A. Meyers and D. G. Shaw

**Variables:**
One temperature: 25 °C
Salinity: 35 g salts/kg sln

**Prepared By:**
P. A. Meyers and D. G. Shaw

Experimental Values
The solubility of hexacosane in seawater was reported to be 10^{-8} \text{g (1/100 g sln and x}_1 = 6 \times 10^{-12}.

**Auxiliary Information**
Method/Apparatus/Procedure:
1 L of a 0.5 g/L solution of the hydrocarbon in acetone was placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:
Analabs, Inc., North Haven, Conn. 99+% pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl_2 sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

**Estimated Error:**
Eight replications were made. The average of the deviations of the mean gave an experimental error of \pm 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.
3. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

Pentane + Seawater 788
Benzene + Seawater E788, 789–791
Methylcyclopentane + Seawater 792
Hexane + Seawater E792, 793
Toluene + Seawater E794, 795–797
Heptane + Seawater E798, 798
α-Xylene + Seawater 799
m-Xylene + Seawater 799
p-Xylene + Seawater 800
Ethylbenzene + Seawater E800, 801
Octane + Seawater E802, 802–803
1,2,3-Trimethylbenzene + Seawater 803
1,2,4-Trimethylbenzene + Seawater 804
Mesitylene + Seawater 804
Cumene + Seawater 805
Nonane + Seawater 805
Naphthalene + Seawater E806, 807–809
Butylbenzene + Seawater 810
sec-Butylbenzene + Seawater 810
tert-Butylbenzene + Seawater 811
Decane + Seawater E811, 812
1-Methylnaphthalene + Seawater 813
Undecane + Seawater 813
Acenaphthene + Seawater 814
Biphenyl + Seawater E814, 815
Dodecane + Seawater E816, 816–817
Fluorene + Seawater 818
Anthracene + Seawater E818, 819
Phenanthrene + Seawater E820, 821–822
Tetradecane + Seawater 822
2-Methylnaphthalene + Seawater 823
1-Methylnaphthalene + Seawater 823
Fluoranthenes + Seawater 824
Pyrene + Seawater E824, 825–826
Hexadecane + Seawater 827
Benz[a]anthracene + Seawater E827, 828
Chrysene + Seawater 829
Octadecane + Seawater 829
Benzo[a]pyrene + Seawater 830
Benzo[e]pyrene + Seawater E830, 831
Eicosane + Seawater 832
Benzo[ghi]perylene + Seawater 832
Benzo[b]triphenylene + Seawater 833
Dibenzo[a,h]anthracene + Seawater 833
Dibenzo[a,j]anthracene + Seawater 834
Hexacosenes + Seawater 834
4. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Formula</th>
<th>Registry Number</th>
<th>Index</th>
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<tbody>
<tr>
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<td>792</td>
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<td>110-54-3</td>
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<tr>
<td>C₆H₁₂</td>
<td>Hexane</td>
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</table>
5. Author Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

Aquan-Yuen, M. E792, 793, E820, 820
Brown, R. L. E788, 789, E794, 795, E800, 801
Button, D. K. E816, 816
Eganhouse, R. P. E806, 807, E814, 815, E820, 821
Fressgarde, M. E798, E802, 802, E811, 812
Gordon, J. E. E806, 807–808
Hatchard, C. G. E792, E798, E802, 802, E811, 812
Hayano, I. E788, 791
Ito, Y. E794, 797
Kito, S. E794, 797
Mackay, D. E788, 789, E792, 793, E794, 795, E820, 820
Parker, C. A. E802, 802, E811, 812
Paul, M. A. E806, 809, E814, 815
Price, L. C. E800, 801, E811, 812
Rossi, S. S. E794, 796, 814, E824, 826
Sada, E. E794, 797
Schwarz, F. P. E806, 809, 813, E818, 819, E820, 822, E824, 826, E830, 831
Shiu, W. Y. E788, 789, E792, 793, E794, 795, E820, 820
Thomas, W. H. E794, 796, 814, E824, 826, 827
Thorne, R. L. E806, 807–808
Umano, S. E788, 791
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