COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES:	**PREPARED BY:**
Temperature: 8.6-31.7°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzo[e]pyrene in water

t/°C	10^8 mol(1) L	10^7 g(1)/100 g sln (compiler)	$10^{10}x_1$ (compiler)
8.6	1.29 ± 0.07	3.25	2.32
14.0	1.42 ± 0.05	3.58	2.56
17.0	1.76 ± 0.13	4.44	3.17
17.5	1.56 ± 0.08	3.94	2.81
20.0	1.82 ± 0.09	4.59	3.28
20.2	1.90 ± 0.14	4.79	3.42
23.0	2.01 ± 0.20	5.07	3.62
23.2	2.12 ± 0.10	5.35	3.82
29.2	2.55 ± 0.02	6.43	4.59
31.7	2.70 ± 0.15	6.81	4.86

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of benzo[e]pyrene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10^7 g(1)/100 g sln
Krasnoshchekova *et al.* (ref 1)	spectral	6	1.79
Schwarz (ref 2)	uv spectral	30	3.32

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.

SOLUBILITY OF BENZO[E]PYRENE (1) IN SEAWATER (2)
TENTATIVE VALUES

T/K	g salts/kg sln	10^7 g(1)/100 g sln
298	6	1.79
298	30	3.32

REFERENCES

1. Krasnoshchekova, R.Ya.; Pakpill, Yu.A; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.

2. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2] (2) Salt Water	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of Benzo[e]pyrene in salt water was reported to be 1.83 µg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.79×10^{-7} g(1)/100 g sln and 1.34×10^{-10} 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 hr and allowed to settle for 16-18 hr. 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:

temp. ± 1°C
soly. ± 0.111
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES:	**PREPARED BY:**
Temperature: 8.9-30.2°C Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of benzo[e]pyrene in 0.5 mol(2)/L

t/°C	10^8 mol(1)/L sln
8.9	0.82
10.8	0.88
15.6	1.01
17.0	1.01
19.2	1.04
21.7	1.13
25.3	1.35
27.1	1.42
30.2	1.66

The corresponding mass percent and mole fraction, x_1, at 25.3°C calculated by the compilers are 3.32×10^{-7} g(1)/100 g sln and 2.44×10^{-10}.

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 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent 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 provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

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:

Solubility ± 19.5% (author)

Temperature ± 0.1°C (author)

REFERENCES: