COMPONENTS:	EVALUATOR:
(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 3-methylcholanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data are available on the solubility of water in 3-methylcholanthrene.

TABLE 1. Quantitative Solubility Studies of 3-Methylcholanthrene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. Unfortunately, the available data, obtained at slightly different temperatures are in poor agreement. Although the values of Mackay and Shiu (ref 2) are generlly more reliable than those of Davis *et al.* (ref 1) the system is not sufficiently well-characterized to justify a preference at this stage and no "best" values have been nominated.

TABLE 2. Reported Solubility Values of 3-Methylcholanthrene (1) in Water (2)

T/K	Reported values[a]	
	10^7 g(1)/100 g sln	10^{10} x_1
298	2.9 (ref 2)	1.9 (ref 2)
300	1.5 (ref 1)	1.0 (ref 1)

a No "best" values nominated because of uncertainties in the available data, see text.

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5] (2) Water; H_2O; [7732-18-5]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
VARIABLES:	**PREPARED BY:**
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylcholanthrene in water

t/°C	10^6 g(1) L^{-1} (2)
27	1.3
	1.8
	1.8

The best value recommended by the authors is 1.5×10^{-6} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.5×10^{-7} g(1)/100 g sln and 1.0×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Hoffman La-Roche; used as received; m.p. range 175.3-177.1°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.3×10^{-6} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylcholanthrene in water at 25°C was reported to be 0.0029 mg(1) dm^{-3} sln and $x_1 = 1.92 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 2.9×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.000021 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES: