



## Project Summary

# FATE, The Environmental Fate Constants Information System Database

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A new online database, designated the FATE database, has been developed for the interactive retrieval of kinetic and equilibrium constants that are needed for assessing the fate of chemicals in the environment. The database contains values for 12 parameters, but may not contain a value for each parameter for each chemical. As of June 1991, the database contained values for about 200 chemicals. Unique features of the database include experimental data that are extracted only from primary references, and pertinent experimental conditions that are entered into the database to assure the user of the credibility and applicability of a value. A newly developed computer program is used to extrapolate hydrolysis rate constants to a standard format. Acidic, basic, and neutral contributions are combined to calculate the overall hydrolysis rate constant,  $k_h$ , and the half-life of the chemical at 25°C and pH7. The data are also reported as second-order acidic and basic rates and a first-order neutral rate at 25°C. Products of transformation are listed for degradation processes when available. A newly developed computerized expert system will be applied to compute accurate fate constant values. The expert system has the capability of crossing chemical boundaries to cover all organic compounds.

*This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).*

### Overview

The FATE database system consists of three data files. The CAS file contains CAS

numbers (Chemical Abstract Service), molecular formulae, SMILES notations (Simplified Molecular Identification and Line Entry System), and chemical and common names. The REF file contains reference numbers and complete citations. The FATES file is cross-referenced to the other files and contains the data for the fate parameters.

The fields for entry of the 12 fate constants in the data base are shown in Table 1.

### Data Sources

The open literature is the source of primary reference for the experimental data included in the FATE database.

Fate constant data for some of the 12 processes are estimated by our staff with computational techniques, using the SMILES notation to define the molecular structure of a chemical. We use the QSAR (Quantitative Structure-Activity Relationships) System and SPARC (SPARC Performs Automated Reasoning in Chemistry) for estimating data.

The QSAR system contains estimation routines that have been modified from published routines. It can be searched by CAS number or SMILES notation and provides the estimated values in a table format.

The expert system SPARC uses computational algorithms based on fundamental chemical structure theory and allows estimation of values for any parameter that depends upon molecular structure. Unlike methods based on property-reactivity correlations, this capability crosses chemical family boundaries to cover all organic compounds. SPARC eventually will contain estimation routines for most, if not all, of the 12 parameters that are included in the FATE database.

A sample report for the hydrolysis rate constant,  $k_h$ , for 1,1,2,2-tetrachloroethane, CAS number [79-34-5] is provided in Figure 1.



Table 1. Entry Fields in FATE Database

Fate code	Symbol	Fate parameter
04	$H_c$	Henry's law constant
05	$k_h$	Hydrolysis rate constant
06	$pK_a$	ionization constant
07	$K_{ow}$	octanol/water partition coefficient
08K	$K_{oc}$	organic-carbon-normalized sediment/water partition coefficient
10	$k_d$	direct (aqueous) photolysis rate constant
11	$K_p$	sediment/water partition coefficient
13	$P_v$	vapor pressure
14	$S_w$	water solubility
21	$\epsilon_a$	molar absorptivity
26	$\phi_r$	aqueous photolysis reaction quantum yield
27	$k_{bio}$	biodegradation rate constant

Fate Data, References as of 12/26/90 Page 1  
 PF7 to scroll backward RETURN to go forward PF3 to abort report

CAS Number: 79345 FATE Code: 05 FATE Reference: C00000165  
 Analytical Method: GLC Estimating Program:  
 Medium: buffered dist. H2O pH: see comments  
 Experimental Temperature: 95.00° C  
 Products: [79-01-6]  
 Comments: 1st order rates were meas. over the pH range 5 to 9 at 11 temp.  
 Data were extrapolated to 1st and 2nd order rates at 25° C with the  
 RATE program. Ea(base) was estimated as 21.2 kcal/mol or 88.8  
 kJ/mol.

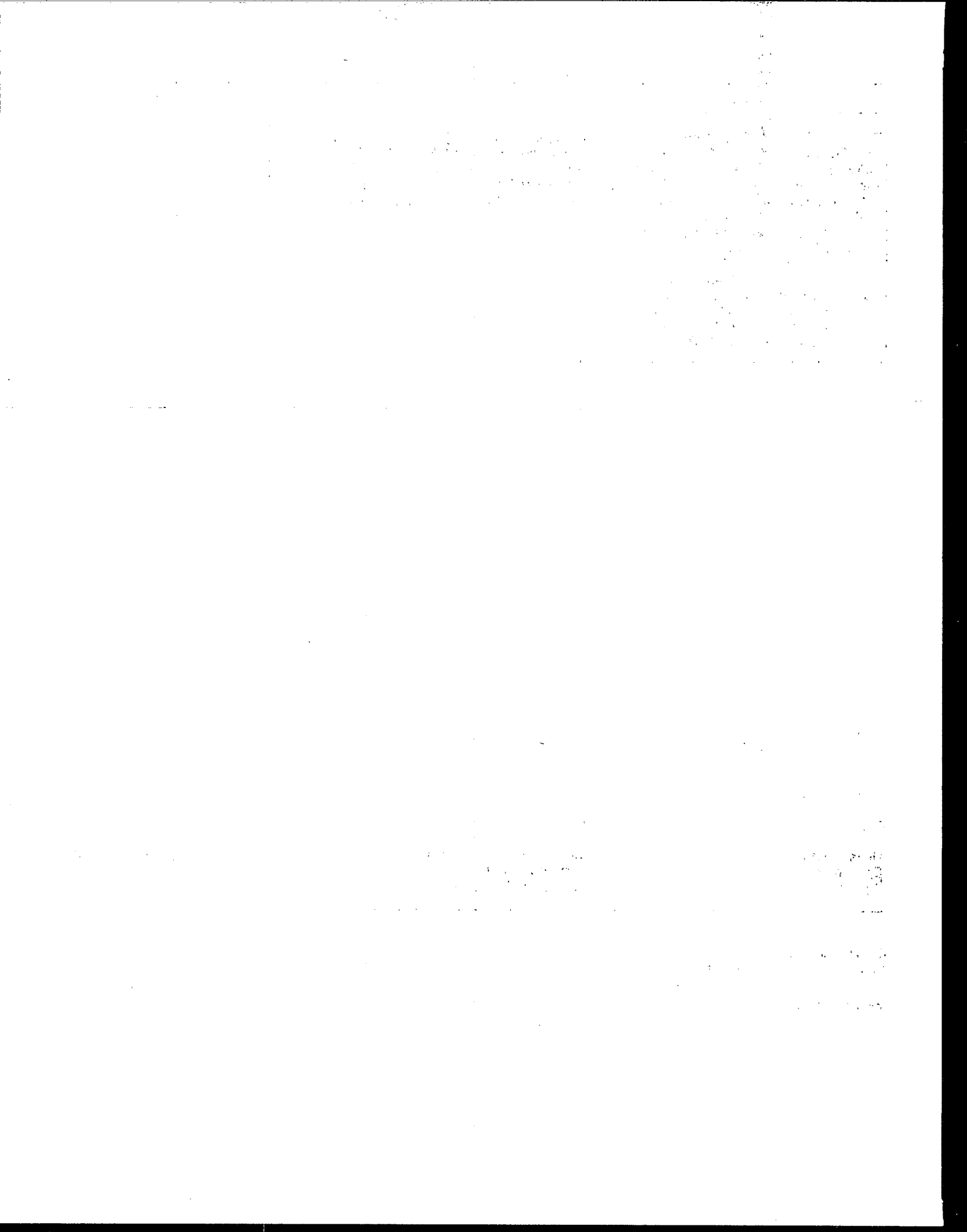
-----Fate Values-----  
 half-life : 98 day (25° C)  
 k(acid) : 0.0/M-yr (25° C)  
 k(base) : 2.6E7/M-yr (25° C)  
 k(h), pH7 : 2.6/yr (25° C)  
 k(neutral) : 0.0/yr (25° C)

Fate Reference: C00000165  
 Authors: Cooper, William J.; Mehran, Mostafa;  
 Flusech, David J.; Joens, Jeffrey A.

Date: 1987  
 Title: Abiotic transformation of halogenated organics. 1. Elimination reaction of 1,1,2,2-tetrachloroethane and formation of 1,1,2-trichloroethene.

Citation: Environ. Sci. Technol. 21(11):1112-1114.

Figure 1. Hydrolysis rate constant report for 1,1,2,2-trichloroethene.



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*National Technical Information Service  
5285 Port Royal Road  
Springfield, VA 22161  
Telephone: 703-487-4650*

*The EPA Project Officer can be contacted at:  
Environmental Research Laboratory  
U.S. Environmental Protection Agency  
Athens, GA 30613-0801*

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