MULTIVARIATE ANALYSIS OF THE INPUT AND OUTPUT DATA IN THE FUGACITY MODEL LEVEL I

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1. Introduction.

QSAR (Quantitative Structure-Activity Relationship) analysis is a well established tool in pharmacology for optimising series of bio-active molecules or understanding a mechanism of activity (Fuller and Marsh, 1972; Fukunaga *et al.*, 1976; Murray *et al.*, 1976; Bonjean and Luu Duc, 1978; Fernandez *et al.*, 1978; Di Paolo *et al.*, 1979; Glennon *et al.*, 1979; Thijssen, 1981; Basak *et al.*, 1983; Reed *et al.*, 1984; Carotti *et al.*, 1985; Noel-Artis *et al.*, 1985; Ray *et al.*, 1985; Goghari *et al.*, 1986; Kawashima *et al.*, 1986; Motoc *et al.*, 1986; Seiler *et al.*, 1986; Werbel *et al.*, 1986; Zeelen, 1986; Basak, 1987; Taillandier and Domard, 1987; Takahashi *et al.*, 1987; Hansch *et al.*, 1989; Dearden, 1990). The technique is statistically-based and aimed at extracting the maximum information from biological data on compounds of known structure and physicochemical properties. Historically, QSAR data analysis was dominated by the use of regression analysis, but since the early 1970s multivariate methods have been increasingly infiltrating the field (Hansch *et al.*, 1973; Moriguchi and Komatsu, 1977; Henry and Block, 1980; Massart-Leën and Massart, 1981; Grassy *et al.*, 1982; Broto *et al.*, 1984; Dunn *et al.*, 1984b; Franke, 1984; Coats *et al.*, 1985; De Flora *et al.*, 1985; de Winter, 1985; Dufton, 1985; Laass, 1985; Leavitt and Mass, 1985; Schaper and Seydel, 1985; Benigni 1986, 1989, 1990; Benigni and Giuliani, 1986, 1987, 1988a, b; Berntsson and Wold, 1986; Lewi, 1986; McFarland and Gans, 1986, 1987; Stouch and Jurs, 1986; Enslein *et al.*, 1987; Mager, 1988; Moreau *et al.*, 1988; Vogt, 1988; Jerman-Blazic *et al.*, 1989; Clementi *et al.*, 1989; Ford *et al.*, 1989; Grassy and Bonnafous, 1989; Livingstone and Rahr, 1989; Rose *et al.*, 1990). Indeed, multivariate methods such as principal component analysis (PCA) or correspondence factor analysis (CFA) can be used to overcome problems of intercorrelations and chance correlation which can appear with multiple regression analysis (Devillers and Lipnick, 1990) or avoid the statistical pitfalls of the Free Wilson (1964) approach (Devillers *et al.*, 1989b; Devillers and Lipnick, 1990; Duewer, 1990). Boolean data (i.e.; 0, 1 or -, +) or classes of activities (e.g.; negative, dubious, and positive) are better analyzed and modeled by means of multivariate approaches (Devillers *et al.*, 1987; Devillers and Chambon, 1989; Borgstedt and Enslein, 1990; Karcher and Devillers, 1990). The graphical displays generated by numerous multivariate techniques are

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particularly suitable to find structure-activity or structure-property relationships (Thioulouse *et al.*, 1991).

In environmental sciences, the same tendency can be noticed to model structure-ecotoxicity relationships. Thus, multivariate analyses are now widely used to structure large collections of data, select training sets, rank chemicals, generate molecular descriptors, compare the sensitivity of different organisms, describe the environmental profiles of the pollutants, and analyze a mechanism of activity (Rose and Jurs, 1982; Burkhard *et al.*, 1983; Dunn *et al.*, 1984a; Enslein *et al.*, 1984; Laurence *et al.*, 1984; Schultz and Moulton, 1985; Stalling *et al.*, 1985a, b; Clarke, 1986; Moulton and Schultz, 1986; Basak *et al.*, 1987, 1988; Brüggemann *et al.*, 1987; McKim *et al.*, 1987a, b, c; Newsted and Giesy, 1987; Niemi *et al.*, 1987; Nirmalakhandan and Speece, 1988; Osterberg *et al.*, 1988; Rauret *et al.*, 1988, 1990; Devillers *et al.*, 1988, 1989; Nendza and Seydel, 1988; Tosato *et al.*, 1988a, b; Veith *et al.*, 1988; Wängberg and Blanck, 1988; Zitko, 1988; Devillers and Doré, 1989; Jonsson *et al.*, 1989; Bradbury *et al.*, 1990; Livingstone, 1989; Eriksson *et al.*, 1990). Recently , we showed too that multivariate analyses were suitable to stress structure-environmental fate relationships (Devillers *et al.*, 1989a; Devillers and Karcher, 1990a). Indeed, the environmental fate and transport of an organic pollutant depend mostly on its basic physicochemical properties. Thus, the aqueous solubility of a chemical controls both the extent to which aquatic biota are exposed to organic toxicants and the potential distribution of these compounds throughout the hydrosphere (Wasik *et al.*, 1983). The volatility of organic compounds is a factor governing their transport through the atmosphere. The vapor pressure of a chemical will determine in part the rate of evaporation from industrial or waste sites as well as the ability to adsorb to particulate matter present in the environment (Wasik *et al.*, 1983). Vapor pressure data can be combined with aqueous solubility data to calculate the Henry's law constant (H) which is needed to estimate vapor exchange rates across the air-water interface (Mackay *et al.*, 1982; Bidleman, 1984; Fendinger and Glotfelty, 1990). The logarithm of the partition coefficient in the n-octanol/water system, log P, is a key physicochemical parameter for characterizing the hydrophobicity of organic compounds. It can be used to predict the bioaccumulation potential and toxicity of organic compounds (Karcher and Devillers; 1990, Lipnick, 1990; Nendza *et al.*, 1990). The human mind is not able to take into account simultaneously the above parameters in order to estimate the theoretical distribution of a chemical between the different compartments of the biosphere (i.e.; air, water, soil, and biota). Mathematical models at different levels of complexity can be used to overcome this problem (Cohen, 1986; McKone and Layton, 1986; Mackay and Paterson, 1989). Among them, the fugacity model level I (Mackay and Paterson, 1981) provides a convenient and accurate simulation tool for preliminary hazard assessment (Bacci and Calamari, 1990). In this model, the input data are the basic physicochemical properties of an organic compound (i.e.; molecular weight, water solubility, log P, and vapor pressure) and the output data can represent the theoretical distribution (in %) of the chemical into the six following compartments: air, water, soil, sediment, suspended sediment, and biota (Mackay and Paterson, 1990). However, with this model, it is difficult to interpret directly the obtained results in terms of structure-environmental fate relationships. To overcome this problem, we proposed to use multivariate approaches for the graphical display and statistical analysis of the output data (Devillers *et al.*, 1989a). Thus, from a data matrix of 29 chemicals, we showed that correspondence factor analysis (CFA) and minimum spanning tree method (MST) were suitable to find structure-environmental distribution relationships. Notice that similar conclusions (Devillers *et al.*, 1989a; Devillers and Karcher, 1990a) were made with 15 chemical distributions obtained by means of the model of Mackay level III (Mackay *et al.*, 1985; Mackay and Paterson,

1990) The scope of the present work is to confirm these preliminary results and try to test the influence of the variability of the inputs on the outputs of the fugacity model level I.

2. Data compilation and calculations

The physicochemical data used in the calculations were obtained from the following report: *Data compilation for chemical fate models* (Devillers *et al.*, 1990). From this report, it is possible to retrieve for each organic pollutant the following information:
- common name
- formula
- CAS Registry number
- molecular weight
- aqueous solubilities in mg/l at specific temperatures with the corresponding bibliographical references (author(s) name(s) and year of publication)
- partition coefficients (log P) at specific temperatures followed by a code which identifies either the type of method used for the determination or the origin of the data:

* D stands for direct method such as shake-flask method, filter probe method, generator column method, etc.
* I stands for indirect method such as chromatography, fragmental approaches, correlation methods, etc.
* C stands for compilation
* R stands for recommended value (i.e.; value selected in a data bank or by an author).
Bibliographical references (author(s) name(s) and year of publication) are also given.

- vapor pressures in Pa at specific temperatures with their corresponding bibliographical references (author(s) name(s) and year of publication).

From this report, 42 chemicals (table 1) were selected so as to present the following criteria:
- recognized and classified as hazardous for environment and human beings
- relevant for QSAR studies (various families and/or functional groups)
- data spanned onto a wide scale
- very high or very low variability in physicochemical data for a same chemical.

The chosen compounds are mainly polyaromatic hydrocarbons (PAH), dioxins, PCBs, and pesticides.
The selection of a value for vapor pressure and aqueous solubility was achieved by first keeping values measured at 25°C and then selecting the most valuable data for QSAR purposes (e.g.; structure and chemical family). If no value measured at 25°C was available, data measured in a 20 to 25°C range were considered. Values measured by the authors themselves were preferred to compilations. For partition coefficient, the selection was based on the same criteria but in addition, values determined in a direct manner were preferentially selected to others.
The selected data for the 42 organic chemicals are marked by an asterisk in table 1.
From these data, the distributions between the six compartments of the biosphere (i.e.; air, water, soil, sediment, suspended sediment, and biota) as defined by Mackay (Mackay *et al.*, 1985; Mackay and Paterson, 1990) were computed on the CFMP software (Devillers and Karcher, 1990b). A correspondence factor analysis was performed on the resulting data (in %) by means of MacMul and GraphMu software (Thioulouse, 1989, 1990).

Table 1. Physicochemical properties for 42 organic pollutants.

N° 1: Acenaphthene

Formula:	**$C_{12}H_{10}$**
CAS Registry Number:	83-32-9
Molecular weight:	154.21
Aqueous solubility:	3.93 mg/l at 25 °C (Mackay and Shiu, 1977) *
	4.16 mg/l at 25 °C (Walters and Luthy, 1984a)
	7.37 mg/l at 25 °C (Banerjee *et al.*, 1980)
	3.88 mg/l at 25 °C (Wauchope and Getzen, 1972)
	3.57 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	3.46 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	4.60 mg/l at 30 °C (Wauchope and Getzen, 1972)
	4.72 mg/l at 30 °C (Wauchope and Getzen, 1972)
	4.76 mg/l at 30 °C (Wauchope and Getzen, 1972)
	4.80 mg/l at 30 °C (Wauchope and Getzen, 1972)
	1.45 mg/l at 0 °C (Wauchope and Getzen, 1972)
log P (octanol-water):	3.92 at 23 °C (D) (Banerjee *et al.*, 1980) *
	4.03 (I) (Walters and Luthy, 1984a)
	3.92 at 20 °C (D) (Veith *et al.*, 1980)
	4.49 (I) (Veith *et al.*, 1980)
	4.45 (I) (Veith *et al.*, 1980)
	4.15 (I) (Mackay *et al.*, 1980)
	4.43 (I) (Arbuckle, 1983)
	4.62 (I) (Arbuckle, 1983)
	3.92 (R) (Sangster, 1989)
	4.03 (I) (Yalkowsky and Valvani, 1979)
	4.33 (I) (Chin *et al.*, 1986)
Vapor pressure:	0.32 Pa at 25 °C (Hine and Mookerjee, 1975)
	0.287 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.37 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.38 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.287 Pa at 25 °C (Wasik *et al.*, 1983) *

N° 2: Aldrin

Formula:	**$C_{12}H_8Cl_6$**
CAS Registry Number:	309-00-2
Molecular weight:	364.91
Aqueous solubility:	0.027 mg/l at 25-30 °C (Park and Bruce, 1968)
	0.017 mg/l at 25 °C (Weil *et al.*, 1974) *
	0.20 mg/l at 25 °C (Richardson and Miller, 1960)
	0.013 mg/l (Kenaga, 1980a, b)
	0.02 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.39 mg/l at 35 °C (Richardson and Miller, 1960)
	0.79 mg/l at 45 °C (Richardson and Miller, 1960)
	0.027 mg/l at 25-29 °C (Martin and Worthing, 1977)
	0.18 mg/l at 25 °C (Biggar and Riggs, 1974)
	0.105 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.35 mg/l at 35 °C (Biggar and Riggs, 1974)
	0.60 mg/l at 45 °C (Biggar and Riggs, 1974)
log P (octanol-water):	3.01 (Lu and Metcalf, 1975)

Table 1 (continued)

	3 (R) (Suntio *et al.*, 1988)
	5.66 (Hawker and Connell, 1986) *
	5.52 (C) (Garten and Trabalka, 1983)
	7.4 (I) (Briggs, 1981)
Vapor pressure:	0.0008 Pa at 20 °C (Edwards, 1966)
	0.005 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.01 Pa at 20 °C (Martin and Worthing, 1977)
	0.019 Pa at 25 °C (Martin and Worthing, 1977) *

N° 3: Anthracene

Formula:	**$C_{14}H_{10}$**
CAS Registry Number:	120-12-7
Molecular weight:	178.23
Aqueous solubility:	0.0446 mg/l at 25 °C (Wasik *et al.*, 1983)
	0.073 mg/l at 25 °C (Mackay and Shiu, 1977) *
	0.0442 mg/l at 25 °C (May *et al.*, 1978a)
	0.0446 mg/l at 25 °C (May *et al.*, 1978b)
	0.0698 mg/l at 25 °C (Walters and Luthy, 1984a)
	0.075 mg/l at 25 °C (Wauchope and Getzen, 1972)
	0.119 mg/l at 35.4 °C (Wauchope and Getzen, 1972)
	0.122 mg/l at 35.4 °C (Wauchope and Getzen, 1972)
	0.123 mg/l at 35.4 °C (Wauchope and Getzen, 1972)
	0.125 mg/l at 35.4 °C (Wauchope and Getzen, 1972)
	0.041 mg/l at 25 °C (Schwarz, 1977)
	0.0233 mg/l at 8.6 °C (Schwarz, 1977)
	0.0244 mg/l at 11.1 °C (Schwarz, 1977)
	0.0257 mg/l at 12.2 °C (Schwarz, 1977)
	0.0274 mg/l at 14 °C (Schwarz, 1977)
	0.0296 mg/l at 15.5 °C (Schwarz, 1977)
	0.0323 mg/l at 18.2 °C (Schwarz, 1977)
	0.0396 mg/l at 20.3 °C (Schwarz, 1977)
	0.0417 mg/l at 23 °C (Schwarz, 1977)
	0.041 mg/l at 23.3 °C (Schwarz, 1977)
	0.0476 mg/l at 26.2 °C (Schwarz, 1977)
	0.0579 mg/l at 28.5 °C (Schwarz, 1977)
	0.0695 mg/l at 31.3 °C (Schwarz, 1977)
	0.030 mg/l at 25 °C (Schwarz and Wasik, 1976)
	0.073 mg/l at 25 °C (Karickhoff *et al.*, 1979)
	0.0557 mg/l at 28.7 °C (May *et al.*, 1978a)
	0.0434 mg/l at 24.6 °C (May *et al.*, 1978a)
	0.0372 mg/l at 22.4 °C (May *et al.*, 1978a)
	0.0291 mg/l at 18.3 °C (May *et al.*, 1978a)
	0.0222 mg/l at 14.1 °C (May *et al.*, 1978a)
	0.0175 mg/l at 10 °C (May *et al.*, 1978a)
	0.0127 mg/l at 5.2 °C (May *et al.*, 1978a)
	0.0570 mg/l at 29 °C (May *et al.*, 1978b)
	0.073 mg/l (Kenaga, 1980a)
log P (octanol-water):	4.69 (I) (Eadsforth, 1986)
	4.51 (I) (Eadsforth, 1986)

Table 1 (continued)

	4.51 (I) (Ghose and Crippen, 1986)
	4.31 (C) (Thomann, 1989)
	4.63 (I) (Yalkowsky and Valvani, 1979)
	3.45 (I) (Veith *et al.*, 1979a)
	4.80 (I) (De Kock and Lord, 1987)
	4.45 (I) (De Kock and Lord, 1987)
	4.73 (I) (Mackay *et al.*, 1980)
	4.45 (I) (Rapaport and Eisenreich, 1984)
	4.63 (I) (Bruggeman *et al.*, 1982)
	4.54 (D) (Karickhoff *et al.*, 1979) *
	4.95 (I) (Klopman *et al.*, 1985)
	4.58 (I) (McDuffie, 1981)
	4.69 (I) (McDuffie, 1981)
	4.59 (I) (Hammers *et al.*, 1982)
	4.20 (I) (D'Amboise and Hanai, 1982)
Vapor pressure:	0.0008 Pa at 25 °C (Wasik *et al.*, 1983)
	0.0008 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00083 Pa at 25 °C (Sonnefeld *et al.*, 1983) *
	0.00049 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00104 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00086 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00111 Pa at 25 °C (Sonnefeld *et al.*, 1983)

N° 4: Benz(a)anthracene (1,2-benzanthracene)

Formula:	$\mathbf{C_{18}H_{12}}$
CAS Registry Number:	56-55-3
Molecular weight:	228.29
Aqueous solubility:	0.0094 mg/l at 25 °C (May *et al.*, 1978b)
	0.014 mg/l at 25 °C (Mackay and Shiu, 1977) *
	0.0168 mg/l at 25 °C (Walters and Luthy, 1984a)
	0.0122 mg/l at 29 °C (May *et al.*, 1978b)
log P (octanol-water):	5.0 (I) (Brooke *et al.*, 1986)
	4.0 (I) (Brooke *et al.*, 1986)
	5.91 (I) (Yalkowsky and Valvani, 1979) *
	6.10 (I) (Mackay *et al.*, 1980)
	5.91 (I) (Walters and Luthy, 1984a)
	5.91 (R) (Sangster, 1989)
Vapor pressure:	0.000028 Pa at 25 °C (Sonnefeld *et al.*, 1983) *
	0.000022 Pa at 25 °C (Sonnefeld *et al.*, 1983)

N° 5: Benzene

Formula:	$\mathbf{C_6H_6}$
CAS Registry Number:	71-43-2
Molecular weight:	78.11
Aqueous solubility:	1780 mg/l at room Temp. (25 +/- 1.5 °C) (McAuliffe, 1963; 1966)
	1790 mg/l at 25 °C (Bohon and Claussen, 1951)
	1755 mg/l at 25 °C (Polak and Lu, 1973)
	1791 mg/l at 25 °C (May *et al.*, 1978b)

Table 1 (continued)

	1770 mg/l at 25 °C (Mackay and Shiu, 1981) *
	1789 mg/l at 25 °C (Wasik *et al.*, 1983)
	820 mg/l at 22 °C (Chiou *et al.*, 1977)
	1696 mg/l at 25 °C (Keeley *et al.*, 1988)
	1750 mg/l at 25 °C (Banerjee *et al.*, 1980)
	1740 mg/l at 21 °C (Chey and Calder, 1972)
	1740 mg/l at 25 °C (Andrews and Keefer, 1949)
	1780 mg/l (Kenaga, 1980a)
	1850 mg/l at 30 °C (Gross and Saylor, 1931)
log P (octanol-water):	2.01 at 25 °C (D) (Schantz and Martire, 1987)
	2.13 (Leo *et al.*, 1971)
	1.56 (Leo *et al.*, 1971)
	2.15 (Leo *et al.*, 1971)
	2.11 (D) (Karickhoff *et al.*, 1979)
	2.12 at 23 °C (D) (Banerjee *et al.*, 1980)
	2.12 at 20 °C (D) (Veith *et al.*, 1980)
	2.13 at 25 °C (D) (Hansch *et al.*, 1968) *
	2.13 at 25 °C (C) (Watarai *et al.*, 1982)
	2.13 (C) (Chiou *et al.*, 1977)
	1.83 (I) (Eadsforth, 1986)
	2.48 (I) (Eadsforth, 1986)
	1.90 (I) (Mackay *et al.*, 1980)
	1.98 (I) (Schantz and Martire, 1987)
	2.13 (I) (Platford, 1979)
	2.15 (I) (Arbuckle, 1983)
	2.24 (I) (Arbuckle, 1983)
	2.34 (I) (Könemann *et al.*, 1979)
	2.13 (R) (Sangster, 1989)
	2.15 (C) (Unger *et al.*, 1978)
	2.39 (I) (Veith *et al.*, 1979a)
	2.15 (I) (Klopman and Iroff, 1981)
	2.17 (I) (Klopman and Iroff, 1981)
	2.13 (I) (Klopman and Iroff, 1981)
	1.97 (I) (Klopman *et al.*, 1985)
	2.10 (I) (Klopman *et al.*, 1985)
	2.33 (I) (Chin *et al.*, 1986)
	2.26 (I) (De Kock and Lord, 1987)
	2.13 (I) (De Kock and Lord, 1987)
	2.25 (I) (Rapaport and Eisenreich, 1984)
	2.48 (I) (Swann *et al.*, 1983)
	2.42 (I) (McDuffie, 1981)
	2.60 (I) (McDuffie, 1981)
	2.23 (I) (Harnisch *et al.*, 1983)
	2.13 (I) (Harnisch *et al.*, 1983)
	2.20 (I) (Hammers *et al.*, 1982)
	2.16 (I) (D'Amboise and Hanai, 1982)
	2.23 (I) (Campbell and Luthy, 1985)
	2.38 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	12688 Pa at 25 °C (Zwolinski and Wilhoit, 1971) *

Table 1 (continued)

	12688 Pa at 25 °C (Hine and Mookerjee, 1975)
	7654 Pa at 14.548 °C (Boublik *et al.*, 1984)
	8962 Pa at 17.72 °C (Boublik *et al.*, 1984)
	10303 Pa at 20.594 °C (Boublik *et al.*, 1984)
	11699 Pa at 23.27 °C (Boublik *et al.*, 1984)
	13817 Pa at 26.886 °C (Boublik *et al.*, 1984)
	16621 Pa at 31.004 °C (Boublik *et al.*, 1984)
	10527 Pa at 21.015 °C (Boublik *et al.*, 1984)
	12431 Pa at 24.549 °C (Boublik *et al.*, 1984)
	16017 Pa at 30.143 °C (Boublik *et al.*, 1984)
	12660 Pa at 25 °C (Bohon and Claussen, 1951)

N° 6: Biphenyl (diphenyl)

Formula:	**$C_{12}H_{10}$**
CAS Registry Number:	92-52-4
Molecular weight:	154.21
Aqueous solubility:	6.708 mg/l at 25 °C (Miller *et al.*, 1984)
	7.0 mg/l at 25 °C (Mackay and Shiu, 1977) *
	6.03 mg/l at 25 °C (Banerjee *et al.*, 1980)
	5.94 mg/l at 25 °C (Andrews and Keefer, 1949)
	7.5 mg/l (Kenaga, 1980a)
	7.48 mg/l at 25 °C (Bohon and Claussen, 1951)
	2.64 mg/l at 0 °C (Wauchope and Getzen, 1972)
	6.96 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	7.13 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	7.29 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	7.35 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	7.08 mg/l at 25 °C (Wauchope and Getzen, 1972)
	8.64 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	8.73 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	8.77 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	8.95 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	8.48 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	8.54 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	8.55 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	8.88 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
log P (octanol-water):	3.76 at 25 °C (D) (Miller *et al.*, 1984)
	3.89 at 25 °C (D) (Woodburn *et al.*, 1984) *
	3.91 (D) (Eadsforth and Moser, 1983)
	4.04 at 23 °C (D) (Banerjee *et al.*, 1980)
	4.09 (Leo *et al.*, 1971)
	4.09 (C) (Thomann, 1989)
	3.16 (Leo *et al.*, 1971)
	4.04 (Leo *et al.*, 1971)
	4.01 (I) (Eadsforth, 1986)
	3.81 (I) (Eadsforth, 1986)
	3.89 (I) (Eadsforth, 1986)
	3.63 (I) (De Kock and Lord, 1987)
	4.0 (I) (De Kock and Lord, 1987)

Table 1 (continued)

	3.75 (I) (Veith *et al.*, 1979a)
	3.79 (I) (Rapaport and Eisenreich, 1984)
	4.10 (I) (Bruggeman *et al.*, 1982)
	4.14 (I) (Mackay *et al.*, 1980)
	4.25 (I) (Arbuckle, 1983)
	4.44 (I) (Arbuckle, 1983)
	3.98 (R) (Sangster, 1989)
	4.03 (I) (Yalkowsky and Valvani, 1979)
	4.10 (C) (Mackay *et al.*, 1982)
	3.90 (R) (Shiu and Mackay, 1986)
	3.70 (I) (Woodburn *et al.*, 1984)
	4.26 (I) (Swann *et al.*, 1983)
	3.91 (I) (McDuffie, 1981)
	4.04 (I) (McDuffie, 1981)
	3.93 (I) (Harnisch *et al.*, 1983)
	3.78 (I) (Harnisch *et al.*, 1983)
	4.08 (I) (Hammers *et al.*, 1982)
	4.05 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	1.19 Pa at 25 °C (Burkhard *et al.*, 1984) *
	0.106 Pa at 5.2 °C (Burkhard *et al.*, 1984)
	0.361 Pa at 14.9 °C (Burkhard *et al.*, 1984)
	1.15 Pa at 24.7 °C (Burkhard *et al.*, 1984)
	1.01 Pa at 25 °C (Burkhard *et al.*, 1985a)

N° 7: Chlordane

Formula:	**$C_{10}H_6Cl_8$**
CAS Registry Number:	57-74-9
Molecular weight:	409.78
Aqueous solubility:	1.85 mg/l at 25 °C (Weil *et al.*, 1974)
	0.009 mg/l at 25 °C (Anonymous, 1988a) *
	0.05 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.056 mg/l (Kenaga, 1980a)
log P (octanol-water):	3.0 (R) (Suntio *et al.*, 1988)
	5.16 (Anonymous, 1988a) *
	6.0 (Hawker and Connell, 1986)
	6.0 (C) (Garten and Trabalka, 1983)
	6.0 (I) (Veith *et al.*, 1979b)
Vapor pressure:	0.00133 Pa at 20 °C (Edwards, 1966)
	0.00133 Pa at 25 °C (Anonymous, 1988a) *
	0.0011 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.00133 Pa at 25 °C (Martin and Worthing, 1977)

N° 8: 2-chlorobiphenyl

Formula:	**$C_{12}H_9Cl$**
CAS Registry Number:	2051-60-7
Molecular weight:	188.66
Aqueous solubility:	5.06 mg/l at 25 °C (Miller *et al.*, 1984) *
	4.13 mg/l at 25 °C (Weil *et al.*, 1974)
log P (octanol-water):	4.50 at 25 °C (D) (Miller *et al.*, 1984) *

Table 1 (continued)

	4.38 at 25 °C (D) (Woodburn *et al.*, 1984)
	4.59 (D) (Bruggeman *et al.*, 1982)
	4.56 (I) (Bruggeman *et al.*, 1982)
	4.10 (I) (McDuffie, 1981)
	4.60 (I) (Rapaport and Eisenreich, 1984)
	4.52 (R) (Sangster, 1989)
	4.30 (R) (Shiu and Mackay, 1986)
	3.75 (I) (Woodburn *et al.*, 1984)
Vapor pressure:	1.53 Pa at 25 °C (Burkhard *et al.*, 1985a) *

N° 9: 1-chlorodibenzo-p-dioxin

Formula:	**$C_{12}H_7ClO_2$**
CAS Registry Number:	39227-53-7
Molecular weight:	218.64
Aqueous solubility:	0.417 mg/l at 25 °C (Shiu et al., 1988) *
	0.136 mg/l at 5°C (Shiu *et al.*, 1988)
	0.233 mg/l at 15 °C (Shiu *et al.*, 1988)
	0.725 mg/l at 35 °C (Shiu *et al.*, 1988)
	1.240 mg/l at 45 °C (Shiu *et al.*, 1988)
log P (octanol-water):	5.30 at 25 °C (I) (Shiu *et al.*, 1988)
	4.97 (I) (Sarna *et al.*, 1984)
	5.20 (I) (Sarna *et al.*, 1984)
	5.25 (I) (Sarna *et al.*, 1984)
	5.05 (I) (Sarna *et al.*, 1984)
	5.18 (I) (Sarna *et al.*, 1984)
	5.23 (I) (Sarna *et al.*, 1984)
	4.75 at 25 °C (R) (Shiu *et al.*, 1988) *
	4.75 (I) (Burkhard and Kuehl, 1986)
	4.2 (I) (Kaiser, 1983)
Vapor pressure:	0.0128 Pa at 25 °C (estimated from Rordorf, 1985) *

N° 10: 2-chlorodibenzo-p-dioxin

Formula:	**$C_{12}H_7ClO_2$**
CAS Registry Number:	39227-54-8
Molecular weight:	218.64
Aqueous solubility:	0.278 mg/l at 25 °C (Shiu *et al.*, 1988)
	0.318 mg/l at 25 °C (Shiu *et al.*, 1988) *
	0.0635 mg/l at 5 °C (Shiu *et al.*, 1988)
	0.137 mg/l at 15 °C (Shiu *et al.*, 1988)
	0.653 mg/l at 35 °C (Shiu *et al.*, 1988)
	1.109 mg/l at 45 °C (Shiu *et al.*, 1988)
	0.133 mg/l at 3.9 °C (Doucette and Andren, 1988)
	0.319 mg/l at 25 °C (Doucette and Andren, 1988)
	0.750 mg/l at 39 °C (Doucette and Andren, 1988)
log P (octanol-water):	4.94 at 25 °C (D) (Shiu *et al.*, 1988)
	5.36 (I) (Sarna *et al.*, 1984)
	5.66 (I) (Sarna *et al.*, 1984)
	5.71 (I) (Sarna *et al.*, 1984)
	5.45 (I) (Sarna *et al.*, 1984)

Table 1 (continued)

	5.64 (I) (Sarna *et al.*, 1984)
	5.69 (I) (Sarna *et al.*, 1984)
	5.00 at 25 °C (R) (Shiu *et al.*, 1988) *
	5.08 (I) (Burkhard and Kuehl, 1986)
	4.2 (I) (Kaiser, 1983)
Vapor pressure:	0.0178 Pa at 25 °C (estimated from Rordorf, 1985) *

N° 11: Chlorpyrifos

Formula:	**$C_9H_{11}Cl_3NO_3PS$**
CAS Registry Number:	2921-88-2
Molecular weight:	350.58
Aqueous solubility:	0.3 mg/l (Kenaga, 1980a,b)
	0.7 mg/l at 19 °C (Bowman and Sans, 1979)
	0.73 mg/l at 20 °C (Bowman and Sans, 1983a,b)
	0.3 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.4 mg/l at 23 °C (Chiou *et al.*, 1977)
	2 mg/l at 35 °C (Martin and Worthing, 1977)
	1.12 mg/l at 24 °C (Felsot and Dahm, 1979) *
log P (octanol-water):	5.11 at 20 °C (D) (Chiou *et al.*, 1977)
	4.96 at 20 °C (D) (Bowman and Sans, 1983b) *
	5.0 (R) (Suntio *et al.*, 1988)
	4.97 (C) (Garten and Trabalka, 1983)
Vapor pressure:	0.0015 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.0025 Pa at 25 °C (Martin and Worthing, 1977) *

N° 12: DDT

Formula:	**$C_{14}H_9Cl_5$**
CAS Registry Number:	50-29-3
Molecular weight:	354.49
Aqueous solubility:	0.0374 mg/l at 25 °C (Babers, 1955)
	0.0012 mg/l at 25 °C (Gunther *et al.*, 1968)
	0.0034 mg/l at 25 °C (Gunther *et al.*, 1968)
	0.025 mg/l at 25 °C (Biggar and Riggs, 1974)
	0.0055 mg/l at 25 °C (Weil *et al.*, 1974)
	0.001 mg/l (Paris *et al.*, 1977)
	0.0023 mg/l at 25 °C (Swann *et al.*, 1983)
	0.0077 mg/l at 20 °C (Friesen *et al.*, 1985)
	0.003 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.017 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.037 mg/l at 35 °C (Biggar and Riggs, 1974)
	0.045 mg/l at 45 °C (Biggar and Riggs, 1974)
	0.0059 mg/l at 2 °C (Babers, 1955)
	0.045 mg/l at 37.5 °C (Babers, 1955)
	0.1 mg/l at 18 °C (Gavaudan and Poussel, 1947)
	0.0031 mg/l at 25 °C (Chiou *et al.*, 1977)
	0.0034 mg/l at 25 °C (Chiou *et al.*, 1977) *
	0.0017 mg/l (Kenaga, 1980a)
log P (octanol-water):	5.3 (I) (Brooke *et al.*, 1986)
	6.19 (C) (Ellgehausen *et al.*, 1980)

Table 1 (continued)

	6.19 (Hawker and Connell, 1986)
	6.19 (C) (Chiou *et al.*, 1977)
	5.56 (I) (Sarna *et al.*, 1984)
	5.51 (I) (Sarna *et al.*, 1984)
	5.45 (I) (Sarna *et al.*, 1984)
	5.65 (I) (Sarna *et al.*, 1984)
	5.49 (I) (Sarna *et al.*, 1984)
	5.44 (I) (Sarna *et al.*, 1984)
	6.0 (R) (Suntio *et al.*, 1988)
	5.44 (I) (Burkhard *et al.*, 1985b)
	6.21 (I) (Eadsforth, 1986)
	6.91 (I) (Eadsforth, 1986)
	6.0 (C) (Thomann, 1989)
	6.17 (D) (Brooke *et al.*, 1986)
	6.16 (D) (Brooke *et al.*, 1986)
	6.22 (D) (Brooke *et al.*, 1986) *
	6.24 (D) (Brooke *et al.*, 1986)
	6.4 (I) (Brooke *et al.*, 1986)
	7.7 (I) (Brooke *et al.*, 1986)
	6.06 (I) (Chin *et al.*, 1986)
	5.76 (C) (Garten and Trabalka, 1983)
	5.63 (I) (De Kock and Lord, 1987)
	6.19 (I) (De Kock and Lord, 1987)
	7.48 (I) (Mackay *et al.*, 1980)
	5.13 (I) (Rapaport and Eisenreich, 1984)
	5.75 (I) (Veith *et al.*, 1979b)
	3.98 (Lu and Metcalf, 1975)
	5.56 (I) (McDuffie, 1981)
	5.63 (I) (McDuffie, 1981)
	6.06 (I) (Harnisch *et al.*, 1983)
	5.84 (I) (Harnisch *et al.*, 1983)
	6.38 (I) (Hammers *et al.*, 1982)
	6.12 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	0.0000293 Pa at 20 °C (Rothman, 1980)
	0.0000573 Pa at 25 °C (Rothman, 1980) *
	0.000124 Pa at 30 °C (Rothman, 1980)
	0.000533 Pa at 40 °C (Rothman, 1980)
	0.0000133 Pa at 20 °C (Edwards, 1966)
	0.000647 Pa at 20 °C (Kuhn and Massini, 1949)
	0.00002 Pa at 20 °C (Balson, 1947)
	0.0000036 Pa at 10 °C (Balson, 1947)
	0.000096 Pa at 30 °C (Balson, 1947)
	0.00043 Pa at 40 °C (Balson, 1947)
	0.00002 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.0000253 Pa at 20 °C (Martin and Worthing, 1977)

N° 13: Dibenzo-p-dioxin

Formula:	**$C_{12}H_8O_2$**
CAS Registry Number:	262-12-4

Table 1 (continued)

Molecular weight:	184.19
Aqueous solubility:	0.842 mg/l at 25 °C (Shiu *et al.*, 1988)
	0.900 mg/l at 25 °C (Shiu *et al.*, 1988) *
	0.205 mg/l at 5 °C (Shiu *et al.*, 1988)
	0.460 mg/l at 15 °C (Shiu *et al.*, 1988)
	1.762 mg/l at 35 °C (Shiu *et al.*, 1988)
	3.262 mg/l at 45 °C (Shiu *et al.*, 1988)
	0.212 mg/l at 4.1 °C (Doucette and Andren, 1988)
	0.901 mg/l at 25 °C (Doucette and Andren, 1988)
	2.394 mg/l at 40 °C (Doucette and Andren, 1988)
log P (octanol-water):	4.37 at 25 °C (D) (Shiu *et al.*, 1988) *
	4.31 (I) (Sarna *et al.*, 1984)
	4.48 (I) (Sarna *et al.*, 1984)
	4.59 (I) (Sarna *et al.*, 1984)
	4.46 (I) (Sarna *et al.*, 1984)
	4.57 (I) (Sarna *et al.*, 1984)
	4.38 (I) (Sarna *et al.*, 1984)
	4.20 (I) (Burkhard and Kuehl, 1986)
	3.40 (I) (Kaiser, 1983)
	4.3 at 25 °C (R) (Shiu *et al.*, 1988)
Vapor pressure:	0.075 Pa at 25 °C (estimated from Rordorf, 1985) *

N° 14: 2,5-dichlorobiphenyl

Formula:	**$C_{12}H_8Cl_2$**
CAS Registry Number:	34883-39-1
Molecular weight:	223.10
Aqueous solubility:	1.94 mg/l at 25 °C (Miller *et al.*, 1984)
	0.58 mg/l at 25 °C (Weil *et al.*, 1974)
	1.12 mg/l at 25 °C (Dunnivant and Elzerman, 1988) *
log P (octanol-water):	5.16 at 25 °C (D) (Miller *et al.*, 1984) *
	5.30 (I) (Rapaport and Eisenreich, 1984)
	5.10 (R) (Shiu and Mackay, 1986)
	5.18 (I) (Bruggeman *et al.*, 1982)
Vapor pressure:	0.0775 Pa at 25 °C (Burkhard *et al.*, 1985a) *

N° 15: 2,7-dichlorodibenzo-p-dioxin

Formula:	**$C_{12}H_6Cl_2O_2$**
CAS Registry Number:	33857-26-0
Molecular weight:	253.08
Aqueous solubility:	0.00375 mg/l at 25 °C (Shiu *et al.*, 1988) *
	0.00109 mg/l at 5 °C (Shiu *et al.*, 1988)
	0.00201 mg/l at 15 °C (Shiu *et al.*, 1988)
	0.00727 mg/l at 35 °C (Shiu *et al.*, 1988)
	0.0134 mg/l at 45 °C (Shiu *et al.*, 1988)
log P (octanol-water):	4.70 (I) (Kaiser, 1983)
	6.28 (I) (Sarna *et al.*, 1984)
	6.64 (I) (Sarna *et al.*, 1984)
	6.72 (I) (Sarna *et al.*, 1984)
	6.38 (I) (Sarna et al., 1984)

Table 1 (continued)

	6.62 (I) (Sarna *et al.*, 1984)
	6.71 (I) (Sarna *et al.*, 1984)
	5.75 at 25 °C (R) (Shiu *et al.*, 1988) *
	5.75 (I) (Burkhard and Kuehl, 1986)
Vapor pressure:	0.00015 Pa at 25 °C (estimated from Rordorf, 1985) *

N° 16: Dichlorvos

Formula:	**$C_4H_7Cl_2O_4P$**
CAS Registry Number:	62-73-7
Molecular weight:	220.98
Aqueous solubility:	10000 mg/l (Kenaga, 1980a)
	8000 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	10000 mg/l at room Temp. (Martin and Worthing, 1977) *
log P (octanol-water):	1.40 (Kenaga and Goring, 1980)
	1.47 at 20 °C (D) (Bowman and Sans, 1983b) *
	1.45 (R) (Suntio *et al.*, 1988)
Vapor pressure:	7 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	1.6 Pa at 20 °C (Martin and Worthing, 1977)
	7.02 Pa at 25 °C (Kim *et al.*, 1984) *

N° 17: Dieldrin

Formula:	**$C_{12}H_8Cl_6O$**
CAS Registry Number:	60-57-1
Molecular weight:	380.91
Aqueous solubility:	< 0.19 mg/l at 25 °C (Lipke and Kearns, 1960)
	0.25 mg/l at 25 °C (Richardson and Miller, 1960)
	0.2 mg/l at 25 °C (Weil *et al.*, 1974)
	0.186 mg/l at 25 - 29 °C (Park and Bruce, 1968)
	0.195 mg/l at 25 °C (Biggar and Riggs, 1974) *
	0.022 mg/l (Kenaga, 1980a)
	0.17 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.14 - 0.18 mg/l at room Temp. (Robeck *et al.*, 1965)
	0.09 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.54 mg/l at 35°C (Richardson and Miller, 1960)
	0.4 mg/l at 35 °C (Biggar and Riggs, 1974)
	1 mg/l at 45 °C (Richardson and Miller, 1960)
	0.65 mg/l at 45 °C (Biggar and Riggs, 1974)
	0.186 mg/l at 25-29 °C (Martin and Worthing, 1977)
log P (octanol-water):	3.7 (R) (Suntio *et al.*, 1988)
	5.48 (Hawker and Connell, 1986)
	5.48 (C) (Thomann, 1989)
	4.49 (D) (Brooke *et al.*, 1986)
	4.51 (D) (Brooke *et al.*, 1986)
	4.55 (D) (Brooke *et al.*, 1986)
	4.60 (D) (Brooke *et al.*, 1986) *
	5.16 (C) (Garten and Trabalka, 1983)
	4.65 (I) (De Kock and Lord, 1987)
	4.51 (I) (De Kock and Lord, 1987)
	6.2 (I) (Briggs, 1981)

Table 1 (continued)

	5.11 (I) (Hammers *et al.*, 1982)
Vapor pressure:	0.000373 Pa at 20 °C (Spencer and Cliath, 1969)
	0.0000133 Pa at 20 °C (Edwards, 1966)
	0.0005 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.0004 Pa at 20 °C (Martin and Worthing, 1977)
	0.00072 Pa at 25 °C (Martin and Worthing, 1977) *

N° 18: Dimethoate

Formula:	**$C_5H_{12}NO_3PS_2$**
CAS Registry Number:	60-51-5
Molecular weight:	229.25
Aqueous solubility:	25000 mg/l (Kenaga, 1980a,b)
	> 5000 mg/l at 20 °C (Bowman and Sans, 1983a)
	20000 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	25000 mg/l at 21 °C (Martin and Worthing, 1977)
	20000 mg/l at 25 °C (Reynolds and Metcalf, 1962) *
log P (octanol-water)	-0.29 (Kenaga and Goring, 1980)
	0.79 at 20 °C (D) (Briggs, 1981)
	0.78 at 20 °C (D) (Bowman and Sans, 1983b) *
	0.8 (R) (Suntio *et al.*, 1988)
	-0.29 (C) (Garten and Trabalka, 1983)
Vapor pressure:	0.01 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.00113 Pa at 25 °C (Martin and Worthing, 1977) *
	0.000674 Pa at 25 °C (Kim *et al.*, 1984)

N° 19: 1,3-dimethylbenzene (m-xylene)

Formula:	**C_8H_{10}**
CAS Registry Number:	108-38-3
Molecular weight:	106.17
Aqueous solubility:	162 mg/l at 25 °C (Polak and Lu, 1973)
	196 mg/l at 25 °C (Bohon and Claussen, 1951)
	173 mg/l at 25 °C (Andrews and Keefer, 1949) *
	146 mg/l at 25 °C (Sutton and Calder, 1975)
	160.32 mg/l at 25 °C (Wasik *et al.*, 1983)
	160.32 mg/l at 25 °C (Tewari *et al.*, 1982)
log P (octanol-water):	3.20 (Leo *et al.*, 1971)
	3.13 at 25 °C (D) (Wasik *et al.*, 1983)
	3.20 at 25 °C (D) (Tewari *et al.*, 1982) *
	3.22 (I) (Eadsforth, 1986)
	3.68 (I) (Eadsforth, 1986)
	3.46 (I) (Eadsforth, 1986)
	3.37 (I) (Haky and Young, 1984)
	3.20 (R) (Sangster, 1989)
	3.29 (I) (Hammers *et al.*, 1982)
Vapor pressure:	1106 Pa at 25 °C (Zwolinski and Wilhoit, 1971) *
	1114 Pa at 25 °C (Hine and Mookerjee, 1975)
	520 Pa at 12.5 °C (Boublik *et al.*, 1984)
	1113 Pa at 25 °C (Boublik *et al.*, 1984)
	1105 Pa at 25 °C (Bohon and Claussen, 1951)

Table 1 (continued)

N° 20: Endrin

Formula:	**$C_{12}H_8Cl_6O$**
CAS Registry Number:	72-20-8
Molecular weight:	380.91
Aqueous solubility:	0.25 mg/l at 25 °C (Biggar and Riggs, 1974)
	0.26 mg/l at 25 °C (Weil *et al.*, 1974)
	0.23 mg/l at 25 °C (Richardson and Miller, 1960)
	0.38 mg/l at 35 °C (Richardson and Miller, 1960)
	0.51 mg/l at 45 °C (Richardson and Miller, 1960)
	0.19 - 0.26 mg/l at room Temp. (Robeck *et al.*, 1965)
	0.024 mg/l (Kenaga, 1980a,b)
	0.24 mg/l at 25 °C (Anonymous, 1988b) *
	0.23 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.13 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.42 mg/l at 35 °C (Biggar and Riggs, 1974)
	0.625 mg/l at 45 °C (Biggar and Riggs, 1974)
log P (octanol-water)	3.2 (R) (Suntio *et al.*, 1988)
	4.56 (C) (Eadsforth, 1986)
	5.01 (I) (Eadsforth, 1986)
	3.56 (I) (Eadsforth, 1986)
	5.34 (Hawker and Connell, 1986)
	5.16 (C) (Garten and Trabalka, 1983)
	4.40 (I) (Rapaport and Eisenreich, 1984)
	5.34 (Anonymous, 1988b) *
Vapor pressure:	0.0000360 Pa at 25 °C (Anonymous, 1988b)
	0.00002 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.0000267 Pa at 25 °C (Martin and Worthing, 1977) *

N° 21: Ethylbenzene

Formula:	**C_8H_{10}**
CAS Registry Number:	100-41-4
Molecular weight:	106.17
Aqueous solubility:	159 mg/l at room Temp. (25 +/- 1.5 °C) (McAuliffe, 1963)
	152 mg/l at room Temp. (25 +/- 1.5 °C) (McAuliffe, 1966)
	177 mg/l at 25 °C (Polak and Lu, 1973)
	208 mg/l at 25 °C (Bohon and Claussen, 1951)
	161.2 mg/l at 25 °C (Sutton and Calder, 1975)
	186.86 mg/l at 25 °C (Wasik *et al.*, 1983) *
	192.27 mg/l at 25 °C (Owens *et al.*, 1986)
	184.74 mg/l at 25 °C (Owens *et al.*, 1986)
	196.41 mg/l at 10 °C (Owens *et al.*, 1986)
	192.38 mg/l at 14 °C (Owens *et al.*, 1986)
	188.56 mg/l at 17 °C (Owens *et al.*, 1986)
	183.14 mg/l at 18 °C (Owens et al , 1986)
	177.94 mg/l at 19 °C (Owens *et al.*, 1986)
	187.92 mg/l at 20 °C (Owens *et al.*, 1986)
	183.04 mg/l at 21 °C (Owens *et al.*, 1986)
	181.87 mg/l at 22 °C (Owens *et al.*, 1986)
	185.90 mg/l at 23.5 °C (Owens *et al.*, 1986)

Table 1 (continued)

	186.12 mg/l at 25.8 °C (Owens *et al.*, 1986)
	185.48 mg/l at 28 °C (Owens *et al.*, 1986)
	188.66 mg/l at 30 °C (Owens *et al.*, 1986)
	193.02 mg/l at 35 °C (Owens *et al.*, 1986)
	152 mg/l at 20 °C (Anonymous, 1988e)
	186.86 mg/l at 25 °C (Tewari *et al.*, 1982)
	168 mg/l at 25 °C (Andrews and Keefer, 1950b)
log P (octanol-water):	3.13 at 25 °C (D) (Wasik *et al.*, 1983) *
	3.13 at 25 °C (D) (Tewari *et al.*, 1982)
	3.13 at 25 °C (D) (Schantz and Martire, 1987)
	3.15 (Leo *et al.*, 1971)
	3.07 (I) (Eadsforth, 1986)
	3.57 (I) (Eadsforth, 1986)
	3.36 (I) (Eadsforth, 1986)
	3.10 (I) (Mackay *et al.*, 1980)
	3.12 (I) (D'Amboise and Hanai, 1982)
	3.14 (I) (Schantz and Martire, 1987)
	3.28 (I) (Campbell and Luthy, 1985)
	3.15 (Anonymous, 1988e)
	3.15 (R) (Sangster, 1989)
	3.16 (I) (Klopman and Iroff, 1981)
	3.21 (I) (Klopman and Iroff, 1981)
	3.13 (I) (Klopman and Iroff, 1981)
	2.95 (I) (Klopman *et al.*, 1985)
	2.75 (I) (Klopman *et al.*, 1985)
	3.30 (I) (Harnisch *et al.*, 1983)
	3.17 (I) (Harnisch *et al.*, 1983)
	3.26 (I) (Hammers *et al.*, 1982)
Vapor pressure:	1266 Pa at 25 °C (Zwolinski and Wilhoit, 1971) *
	1276 Pa at 25 °C (Hine and Mookerjee, 1975)
	933 Pa at 20 °C (Anonymous, 1988e)
	1333 Pa at 25.88 °C (Boublik *et al.*, 1984)
	1266 Pa at 25 °C (Bohon and Claussen, 1951)

N° 22: Fluoranthene

Formula:	$C_{16}H_{10}$
CAS Registry Number:	206-44-0
Molecular weight:	202.26
Aqueous solubility:	0.206 mg/l at 25 °C (May *et al.*, 1978b) *
	0.260 mg/l at 25 °C (Mackay and Shiu, 1977)
	0.199 mg/l at 25 °C (Walters and Luthy, 1984a)
	0.236 mg/l at 25 °C (Schwarz and Wasik, 1976)
	0.264 mg/l at 29 °C (May *et al.*, 1978b)
log P (octanol-water):	5.20 (Scheele, 1980) *
	5.22 (I) (Yalkowsky and Valvani, 1979)
	5.22 (I) (Walters and Luthy, 1984a,b)
	5.22 (I) (Miller *et al.*, 1985)
	5.29 (I) (Mackay *et al.*, 1980)
	5.20 (R) (Sangster, 1989)

Table 1 (continued)

	4.84 (I) (Chin *et al.*, 1986)
	5.22 (I) (Bruggeman *et al.*, 1982)
	4.47 (I) (Harnisch *et al.*, 1983)
	4.31 (I) (Harnisch *et al.*, 1983)
Vapor pressure:	0.00123 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00124 Pa at 25 °C (Wasik *et al.*, 1983) *

N° 23: Fluorene

Formula:	**$C_{13}H_{10}$**
CAS Registry Number:	86-73-7
Molecular weight:	166.22
Aqueous solubility:	1.685 mg/l at 25 °C (May *et al.*, 1978b)
	1.90 mg/l at 25 °C (Wauchope and Getzen, 1972) *
	0.66 mg/l at 0 °C (Wauchope and Getzen, 1972)
	1.86 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	1.87 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	1.88 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	2.33 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	2.34 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	2.37 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	2.41 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	2.10 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	2.23 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	2.25 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	1.98 mg/l at 25 °C (Mackay and Shiu, 1977)
	1.90 mg/l at 25 °C (Walters and Luthy, 1984a)
	2.04 mg/l at 30 °C (Yalkowsky *et al.*, 1983)
	1.68 mg/l at 25 °C (Wasik *et al.*, 1983)
log P (octanol-water):	4.18 at 30 °C (D) (Yalkowsky *et al.*, 1983)
	4.18 (I) (Bruggeman *et al.*, 1982)
	4.27 (I) (Mackay *et al.*, 1980)
	4.34 (I) (Yalkowsky *et al.*, 1983)
	4.18 (R) (Sangster, 1989) *
	4.47 (I) (Yalkowsky and Valvani, 1979)
	4.10 (I) (Chin *et al.*, 1986)
	4.23 (I) (Rapaport and Eisenreich, 1984)
	4.63 (I) (Klopman *et al.*, 1985)
	4.17 (I) (Hammers *et al.*, 1982)
Vapor pressure:	0.08 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.08 Pa at 25 °C (Wasik *et al.*, 1983)
	0.088 Pa at 25 °C (Sonnefeld *et al.*, 1983) *
	0.127 Pa at 25 °C (Sonnefeld *et al.*, 1983)

N° 24: Heptachlor

Formula:	**$C_{10}H_5Cl_7$**
CAS Registry Number:	76-44-8
Molecular weight:	373.32
Aqueous solubility:	0.18 mg/l at 25 °C (Biggar and Riggs, 1974)
	0.03 mg/l (Kenaga, 1980a,b)

Table 1 (continued)

	0.056 mg/l at 25 - 30 °C (Park and Bruce, 1968)
	0.056 mg/l at 25 °C (Anonymous, 1988c) *
	0.1 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.1 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.315 mg/l at 35 °C (Biggar and Riggs, 1974)
	0.49 mg/l at 45 °C (Biggar and Riggs, 1974)
	0.056 mg/l at 25-29 °C (Martin and Worthing, 1977)
log P (octanol-water):	3.9 (R) (Suntio *et al.*, 1988)
	3.87 (Anonymous, 1988c)
	5.38 (Hawker and Connell, 1986) *
	5.38 (C) (Thomann, 1989)
	5.44 (C) (Garten and Trabalka, 1983)
	5.58 (I) (De Kock and Lord, 1987)
	5.5 (I) (De Kock and Lord, 1987)
	5.44 (I) (Veith *et al.*, 1979b)
	5.27 (I) (McDuffie, 1981)
Vapor pressure:	0.04 Pa at 20 °C (Edwards, 1966)
	0.040 Pa at 25 °C (Anonymous, 1988c) *
	0.03 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.04 Pa at 25 °C (Martin and Worthing, 1977)

N° 25: Heptachlor epoxide

Formula:	**$C_{10}H_5Cl_7O$**
CAS Registry Number:	1024-57-3
Molecular weight:	389.32
Aqueous solubility:	0.35 mg/l at 25 °C (Anonymous, 1988c) *
	0.35 mg/l at 25 °C (Weil *et al.*, 1974)
	0.20 mg/l at 25 °C (Biggar and Riggs, 1974)
	0.11 mg/l at 15 °C (Biggar and Riggs, 1974)
	0.35 mg/l at 35 °C (Biggar and Riggs, 1974)
	0.60 mg/l at 45 °C (Biggar and Riggs, 1974)
	0.35 mg/l at 25-29 °C (Park and Bruce, 1968)
log P (octanol-water):	2.65 (Anonymous, 1988c)
	4.43 (Anonymous, 1988c)
	5.40 (Anonymous, 1988c)
	5.39 (Hawker and Connell, 1986) *
	5.4 (C) (Thomann, 1989)
	5.40 (C) (Garten and Trabalka, 1983)
	5.40 (I) (Veith *et al.*, 1979b)
Vapor pressure:	0.040 Pa at 25 °C (Anonymous, 1988c) *

N° 26: Hexachlorobenzene

Formula:	**C_6Cl_6**
CAS Registry Number:	118-74-1
Molecular weight:	284.78
Aqueous solubility:	0.005 mg/l at 25 °C (Anonymous, 1988f) *
	0.047 mg/l at 25 °C (Miller *et al.*, 1984)
	0.0049 mg/l (Yalkowsky and Valvani, 1981)
	0.005 mg/l at 25 °C (Weil *et al.*, 1974)

Table 1 (continued)

	0.035 mg/l (Kenaga, 1980a)
log P (octanol-water):	5.8 (Anonymous, 1988f)
	5.47 at 25 °C (D) (Miller *et al.*, 1984) *
	5.31 at 25 °C (D) (Watarai *et al.*, 1982)
	5.02 (D) (Harnisch *et al.*, 1983)
	5.20 (D) (Harnisch *et al.*, 1983)
	5.41 (D) (Harnisch *et al.*, 1983)
	5.51 (D) (Harnisch *et al.*, 1983)
	5.55 (D) (Harnisch *et al.*, 1983)
	5.66 (D) (Harnisch *et al.*, 1983)
	5.92 (D) (Harnisch *et al.*, 1983)
	6.86 (I) (Burkhard *et al.*, 1985b)
	6.42 (I) (Burkhard *et al.*, 1985b)
	6.41 (I) (Eadsforth, 1986)
	5.48 (I) (Ghose and Crippen, 1986)
	5.5 (C) (Thomann, 1989)
	5.5 (C) (Yalkowsky and Valvani, 1981)
	6.6 (I) (Brooke *et al.*, 1986)
	5.9 (I) (Brooke *et al.*, 1986)
	6.51 (I) (Chin *et al.*, 1986)
	6.27 (I) (Könemann *et al.*, 1979)
	6.92 (I) (De Kock and Lord, 1987)
	7.42 (I) (Veith *et al.*, 1979a)
	5.23 (I) (Veith *et al.*, 1979b)
	5.44 at 20 °C (D) (Briggs, 1981)
	4.13 (Lu and Metcalf, 1975)
	6.47 (I) (McDuffie, 1981)
	5.46 (I) (Harnisch *et al.*, 1983)
	5.26 (I) (Harnisch *et al.*, 1983)
	5.66 (I) (Hammers *et al.*, 1982)
	6.38 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	0.0022 Pa at 25 °C (Anonymous, 1988f) *
	0.0015 Pa at 20 °C (Anonymous, 1988f)
	0.0015 Pa at 20 °C (Martin and Worthing, 1977)

N° 27: 2,2',4,4',6,6'-hexachlorobiphenyl

Formula:	**$C_{12}H_4Cl_6$**
CAS Registry Number:	33979-03-2
Molecular weight:	360.88
Aqueous solubility:	0.00041 mg/l at 25 °C (Miller *et al.*, 1984) *
	0.0009 mg/l at 25 °C (Weil *et al.*, 1974)
	0.0023 mg/l at 25 °C (Dunnivant and Elzerman, 1988)
log P (octanol-water):	7.55 at 25 °C (D) (Miller *et al.*, 1984) *
	6.39 (I) (Burkhard *et al.*, 1985b)
	8.31 (I) (Burkhard *et al.*, 1985b)
	7.75 (Hawker and Connell, 1986)
	6.10 (C) (Garten and Trabalka, 1983)
	7.00 (R) (Shiu and Mackay, 1986)
	7.12 (I) (Bruggeman *et al.*, 1982)

Table 1 (continued)

	6.37 (I) (McDuffie, 1981)
	6.41 (I) (McDuffie, 1981)
Vapor pressure:	0.00173 Pa at 25 °C (Burkhard *et al.*, 1985a) *
N° 28: Malathion	
Formula:	**$C_{10}H_{19}O_6PS_2$**
CAS Registry Number:	121-75-5
Molecular weight:	330.35
Aqueous solubility:	145 mg/l (Kenaga, 1980a,b)
	143 mg/l at 20 °C (Bowman and Sans, 1983a,b)
	145 mg/l at 20 °C (R) (Suntio *et al.*, 1988) *
	145 mg/l at 20 °C (Chiou *et al.*, 1977)
	145 mg/l at room Temp. (Martin and Worthing, 1977)
log P (octanol-water):	2.89 at 20 °C (D) (Chiou *et al.*, 1977)
	2.84 at 20 °C (D) (Bowman and Sans, 1983b) *
	2.8 (R) (Suntio *et al.*, 1988)
	2.9 (C) (Thomann, 1989)
	2.89 (C) (Garten and Trabalka, 1983)
	3.61 (I) (Mackay *et al.*, 1980)
Vapor pressure:	0.0011 Pa at 25 °C (Kim *et al.*, 1984) *
	0.001 Pa at 20 °C (R) (Suntio *et al.*, 1988)
N° 29: Methomyl	
Formula:	**$C_5H_{10}N_2O_2S$**
CAS Registry Number:	16752-77-5
Molecular weight:	162.21
Aqueous solubility:	10000 mg/l (Kenaga, 1980a)
	10000 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	58000 mg/l at 25 °C (Martin and Worthing, 1977) *
	> 1000 mg/l at 20 °C (Bowman and Sans, 1983a)
log P (octanol-water):	0.13 at 20 °C (D) (Bowman and Sans, 1983b) *
	0.2 (R) (Suntio *et al.*, 1988)
Vapor pressure:	0.004 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.00667 Pa at 25 °C (Martin and Worthing, 1977) *
N° 30: Monuron	
Formula:	**$C_9H_{11}ClN_2O$**
CAS Registry Number:	150-68-5
Molecular weight:	198.65
Aqueous solubility:	230 mg/l at 25 °C (Bailey and White, 1965) *
	200 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	230 mg/l (Kenaga, 1980a)
	230 mg/l at 25 °C (Martin and Worthing, 1977)
log P (octanol-water):	2.08 (D) (Ellgehausen *et al.*, 1980) *
	1.8 (R) (Suntio *et al.*, 1988)
Vapor pressure:	0.003 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.0000667 Pa at 25 °C (Martin and Worthing, 1977) *

Table 1 (continued)

N° 31: Naphthalene

Formula:	**$C_{10}H_8$**
CAS Registry Number:	91-20-3
Molecular weight:	128.17
Aqueous solubility:	31.69 mg/l at 25 °C (May *et al.*, 1978b) *
	30 mg/l at 25 °C (Schwarz and Wasik, 1977)
	24.35 mg/l at 18 °C (Schwarz and Wasik, 1977)
	20.12 mg/l at 12 °C (Schwarz and Wasik, 1977)
	30.25 mg/l at 25 °C (Schwarz, 1977)
	17.94 mg/l at 8.4 °C (Schwarz, 1977)
	19.10 mg/l at 11.1 °C (Schwarz, 1977)
	21.28 mg/l at 14 °C (Schwarz, 1977)
	24.10 mg/l at 17.5 °C (Schwarz, 1977)
	26.53 mg/l at 20.2 °C (Schwarz, 1977)
	28.45 mg/l at 23.2 °C (Schwarz, 1977)
	31.79 mg/l at 26.3 °C (Schwarz, 1977)
	34.35 mg/l at 29.2 °C (Schwarz, 1977)
	36.27 mg/l at 31.8 °C (Schwarz, 1977)
	31.2 mg/l at 25 °C (Wauchope and Getzen, 1972)
	13.7 mg/l at 0 °C (Wauchope and Getzen, 1972)
	28.3 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	28.8 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	29.1 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	30.7 mg/l at 24.5 °C (Wauchope and Getzen, 1972)
	37.3 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	38.1 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	38.2 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	38.3 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	37.6 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	37.8 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	38.1 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	31.7 mg/l at 25 °C (Mackay and Shiu, 1977)
	30.63 mg/l at 25 °C (Wasik *et al.*, 1983)
	32.9 mg/l at 25 °C (Walters and Luthy, 1984a)
	31.7 mg/l at 25 °C (Karickhoff *et al.*, 1979)
	34.4 mg/l at 25 °C (Bohon and Claussen, 1951)
	33.58 mg/l at 25 °C (Gordon and Thorne, 1967)
	31.7 mg/l (Kenaga, 1980a)
	31.5 mg/l at 25 °C (Andrews and Keefer, 1949)
	30 mg/l at room Temp. (Martin and Worthing, 1977)
log P (octanol-water):	3.35 (I) (Bruggeman *et al.*, 1982)
	3.35 at 25 °C (D) (Wasik *et al.*, 1983) *
	3.36 at 20 °C (D) (Briggs, 1981)
	3.36 (D) (Karickhoff *et al.*, 1979)
	3.17 (I) (Veith *et al.*, 1979a)
	3.30 (I) (Mackay *et al.*, 1980)
	3.43 (I) (Eadsforth, 1986)
	3.65 (I) (Campbell and Luthy, 1985)
	3.01 (I) (Eadsforth, 1986)

Table 1 (continued)

	3.3 (C) (Thomann, 1989)
	3.37 (C) (Chiou *et al.*, 1977)
	3.23 (D) (Brooke *et al.*, 1986)
	3.24 (D) (Brooke *et al.*, 1986)
	3.26 (D)(Brooke *et al.*, 1986)
	3.28 (D) (Brooke *et al.*, 1986)
	3.35 (R) (Sangster, 1989)
	3.35 (I) (Yalkowsky and Valvani, 1979)
	3.36 (I) (De Kock and Lord, 1987)
	3.35 (D) (Opperhuizen, 1987)
	3.26 (I) (Rapaport and Eisenreich, 1984)
	3.40 (I) (Miller *et al.*, 1984)
	3.52 (I) (Klopman *et al.*, 1985)
	3.40 (I) (McDuffie, 1981)
	3.54 (I) (McDuffie, 1981)
	3.45 (I) (Hammers *et al.*, 1982)
	3.18 (I) (D'Amboise and Hanai, 1982)
	3.35 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	11.20 Pa at 25 °C (Hine and Mookerjee, 1975)
	10.4 Pa at 25 °C (Sonnefeld *et al.*, 1983) *
	10.4 Pa at 25 °C (Wasik *et al.*, 1983)
	10.8 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	12.3 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	6.56 Pa at 20 °C (Martin and Worthing, 1977)
N° 32: Nitrobenzene	
Formula:	**$C_6H_5NO_2$**
CAS Registry Number:	98-95-3
Molecular weight:	123.11
Aqueous solubility:	2093 mg/l at 25 °C (Banerjee *et al.*, 1980) *
	3828.7 mg/l at 25 °C (Tewari *et al.*, 1982)
	1780 mg/l (Kenaga, 1980a)
	2050 mg/l at 30 °C (Gross and Saylor, 1931)
	1780 mg/l at 15 °C (Gross and Saylor, 1931)
	1930 mg/l at 25 °C (Andrews and Keefer, 1950a)
log P (octanol-water):	1.83 at 23 °C (D) (Banerjee *et al.*, 1980)
	1.85 (Leo *et al.*, 1971)
	1.79 (Lu and Metcalf, 1975)
	1.85 at 20 °C (D) (Briggs, 1981)
	1.85 at 25 °C (D) (Tewari *et al.*, 1982) *
	1.88 (Leo *et al.*, 1971)
	1.70 (I) (Hammers *et al.*, 1982)
	1.82 (I) (Veith *et al.*, 1979a)
	1.83 at 20 °C (D) (Veith *et al.*, 1980)
	1.87 (I) (Veith *et al.*, 1980)
	1.83 (I) (Arbuckle, 1983)
	1.84 (I) (Arbuckle, 1983)
	1.84 (I) (Campbell and Luthy, 1985)
	1.85 (R) (Sangster, 1989)

Table 1 (continued)

	1.85 at 25 °C (D) (Hansch *et al.*, 1968)
	2.15 (I) (Klopman *et al.*, 1985)
	1.78 (I) (McDuffie, 1981)
Vapor pressure:	37.86 Pa at 25 °C (Hine and Mookerjee, 1975) *

N° 33: Octachlorodibenzo-p-dioxin

Formula:	**$C_{12}Cl_8O_2$**
CAS Registry Number:	3268-87-9
Molecular weight:	459.75
Aqueous solubility:	0.000000074 mg/l at 25 °C (Shiu *et al.*, 1988) *
	0.0000004 mg/l at 20 °C (Friesen *et al.*, 1985)
	0.000002 mg/l at 40 °C (Friesen *et al.*, 1985)
	0.00000031 mg/l at 40 °C (Doucette and Andren, 1988)
log P (octanol-water):	7.59 at 25 °C (D) (Shiu *et al.*, 1988)
	8.20 at 25 °C (R) (Shiu *et al.*, 1988) *
	12.21 (I) (Sarna *et al.*, 1984)
	12.60 (I) (Sarna *et al.*, 1984)
	12.97 (I) (Sarna *et al.*, 1984)
	11.82 (I) (Sarna *et al.*, 1984)
	12.72 (I) (Sarna *et al.*, 1984)
	13.08 (I) (Sarna *et al.*, 1984)
	8.60 (I) (Burkhard and Kuehl, 1986)
Vapor pressure:	1.1 E-10 Pa at 25 °C (estimated from Rordorf, 1985) *

N° 34: Phenanthrene

Formula:	**$C_{14}H_{10}$**
CAS Registry Number:	85-01-8
Molecular weight:	178.23
Aqueous solubility:	1.002 mg/l at 25 °C (May *et al.*, 1978a,b) *
	1.00 mg/l at 25 °C (Wasik *et al.*, 1983)
	1.29 mg/l at 25 °C (Mackay and Shiu, 1977)
	1.15 mg/l at 25 °C (Schwarz, 1977)
	0.501 mg/l at 8.4 °C (Schwarz, 1977)
	0.551 mg/l at 11.1 °C (Schwarz, 1977)
	0.64 mg/l at 14 °C (Schwarz, 1977)
	0.784 mg/l at 17.5 °C (Schwarz, 1977)
	0.88 mg/l at 20.2 °C (Schwarz, 1977)
	1.085 mg/l at 23.3 °C (Schwarz, 1977)
	1.372 mg/l at 29.3 °C (Schwarz, 1977)
	1.627 mg/l at 31.8 °C (Schwarz, 1977)
	1.18 mg/l at 25 °C (Wauchope and Getzen, 1972)
	0.39 mg/l at 0 °C (Wauchope and Getzen, 1972)
	1.11 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	1.12 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	1.16 mg/l at 24.6 °C (Wauchope and Getzen, 1972)
	1.49 mg/l at 29.9 °C (Wauchope and Getzen, 1972)
	1.47 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	1.48 mg/l at 30.3 °C (Wauchope and Getzen, 1972)
	1.52 mg/l at 30.3 °C (Wauchope and Getzen, 1972)

Table 1 (continued)

	0.994 mg/l at 25 °C (Andrews and Keefer, 1949)
	1.29 mg/l at 25 °C (Walters and Luthy, 1984a)
	1.29 mg/l at 25 °C (Karickhoff *et al.*, 1979)
	1.277 mg/l at 29.9 °C (May *et al.*, 1978a)
	0.995 mg/l at 24.3 °C (May *et al.*, 1978a)
	0.816 mg/l at 21 °C (May *et al.*, 1978a)
	0.601 mg/l at 15 °C (May *et al.*, 1978a)
	0.512 mg/l at 12.5 °C (May *et al.*, 1978a)
	0.468 mg/l at 10 °C (May *et al.*, 1978a)
	0.423 mg/l at 8.5 °C (May *et al.*, 1978a)
	1.220 mg/l at 29 °C (May *et al.*, 1978b)
	1.29 mg/l (Kenaga, 1980a)
log P (octanol-water):	4.52 (D) (Eadsforth and Moser, 1983) *
	4.57 (D) (Karickhoff *et al.*, 1979)
	4.28 (I) (Haky and Young, 1984)
	4.31 (I) (Eadsforth and Moser, 1983)
	4.64 (I) (Mackay *et al.*, 1980)
	4.52 (R) (Sangster, 1989)
	4.63 (I) (Yalkowsky and Valvani, 1979)
	4.39 (I) (Chin *et al.*, 1986)
	4.60 (Leo *et al.*, 1976)
	4.46 (Leo *et al.*, 1971)
	4.63 (I) (Bruggeman *et al.*, 1982)
	4.95 (I) (Klopman *et al.*, 1985)
	4.45 (I) (McDuffie, 1981)
	4.56 (I) (McDuffie, 1981)
	4.42 (I) (Hammers *et al.*, 1982)
Vapor pressure:	0.0161 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.0161 Pa at 25 °C (Wasik *et al.*, 1983)
	0.0227 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.0187 Pa at 25 °C (Sonnefeld *et al.*, 1983) *

N° 35: Phorate

Formula:	$C_7H_{17}O_2PS_3$
CAS Registry Number:	298-02-2
Molecular weight:	260.36
Aqueous solubility:	85 mg/l at 25 °C (Reynolds and Metcalf, 1962)
	50 mg/l (Kenaga, 1980a)
	20 mg/l at 24 °C (Felsot and Dahm, 1979)
	17.9 mg/l at 20 °C (Bowman and Sans, 1979; 1983b)
	40 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	19.2 mg/l at 25 °C (Lord and Burt, 1964)
	50 mg/l at Room Temp. (Martin and Worthing, 1977) *
log P (octanol-water):	3.33 (D) (Felsot and Dahm, 1979)
	4.26 at 20 °C (D) (Briggs, 1981)
	3.83 at 20 °C (D) (Bowman and Sans, 1983b) *
	3.8 (R) (Suntio *et al.*, 1988)
Vapor pressure:	0.0738 Pa at 25 °C (Kim *et al.*, 1984) *
	0.1 Pa at 20 °C (R) (Suntio *et al.*, 1988)

Table 1 (continued)

	0.112 Pa at 20 °C (Martin and Worthing, 1977)

N° 36: Pyrene

Formula:	**$C_{16}H_{10}$**
CAS Registry Number:	129-00-0
Molecular weight:	202.26
Aqueous solubility:	0.132 mg/l at 25 °C (May *et al.*, 1978b)
	0.129 mg/l at 25 °C (Schwarz, 1977) *
	0.0546 mg/l at 12.2 °C (Schwarz, 1977)
	0.0686 mg/l at 15.5 °C (Schwarz, 1977)
	0.079 mg/l at 17.4 °C (Schwarz, 1977)
	0.0924 mg/l at 20.3 °C (Schwarz, 1977)
	0.117 mg/l at 23 °C (Schwarz, 1977)
	0.118 mg/l at 23.3 °C (Schwarz, 1977)
	0.144 mg/l at 26.2 °C (Schwarz, 1977)
	0.145 mg/l at 26.7 °C (Schwarz, 1977)
	0.164 mg/l at 28.5 °C (Schwarz, 1977)
	0.188 mg/l at 31.3 °C (Schwarz, 1977)
	0.148 mg/l at 25 °C (Wauchope and Getzen, 1972)
	0.049 mg/l at 0 °C (Wauchope and Getzen, 1972)
	0.124 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	0.128 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	0.129 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	0.130 mg/l at 22.2 °C (Wauchope and Getzen, 1972)
	0.228 mg/l at 34.5 °C (Wauchope and Getzen, 1972)
	0.235 mg/l at 34.5 °C (Wauchope and Getzen, 1972)
	0.133 mg/l at 25 °C (Walters and Luthy, 1984a)
	0.162 mg/l at 29 °C (May *et al.*, 1978b)
	0.135 mg/l (Kenaga, 1980a)
	0.135 mg/l at 25 °C (Mackay and Shiu, 1977)
log P (octanol-water):	5.18 (D) (Karickhoff *et al.*, 1979) *
	4.50 (I) (D'Amboise and Hanai, 1982)
	5.12 (I) (Mackay *et al.*, 1980)
	5.52 (I) (Burkhard *et al.*, 1985b)
	4.95 (I) (Burkhard *et al.*, 1985b)
	5.00 (R) (Sangster, 1989)
	5.22 (I) (Yalkowsky and Valvani, 1979)
	4.97 (I) (Chin *et al.*, 1986)
	4.96 (I) (Rapaport and Eisenreich, 1984)
	5.22 (I) (Bruggeman *et al.*, 1982)
	5.60 (I) (Klopman *et al.*, 1985)
	5.04 (I) (McDuffie, 1981)
	5.13 (I) (McDuffie, 1981)
	5.09 (Means *et al.*, 1980)
	4.93 (I) (Hammers *et al.*, 1982)
Vapor pressure:	0.0006 Pa at 25 °C (Sonnefeld *et al.*, 1983) *
	0.0006 Pa at 25 °C (Wasik *et al.*, 1983)
	0.00088 Pa at 25 °C (Sonnefeld *et al.*, 1983)
	0.00027 Pa at 25 °C (Sonnefeld *et al.*, 1983)

Table 1 (continued)

N° 37: Ronnel (fenchlorphos)

Formula:	**$C_8H_8Cl_3O_3PS$**
CAS Registry Number:	299-84-3
Molecular weight:	321.54
Aqueous solubility:	44 mg/l at 25 °C (Gunther *et al.*, 1968)
	6 mg/l (Kenaga, 1980a,b)
	1.08 mg/l at 20 °C (Chiou *et al.*, 1977) *
	0.6 mg/l at 20 °C (Bowman and Sans, 1979)
	0.6 mg/l at 20 °C (Bowman and Sans, 1983b)
	1 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	40 mg/l at room Temp. (Martin and Worthing, 1977)
log P (octanol-water):	4.88 at 20 °C (D) (Chiou *et al.*, 1977) *
	4.81 at 20 °C (D) (Bowman and Sans, 1983b)
	4.8 (R) (Suntio *et al.*, 1988)
	4.88 (C) (Garten and Trabalka, 1983)
Vapor pressure:	0.01 Pa at 20 °C (R) (Suntio *et al.*, 1988)
	0.107 Pa at 25 °C (Martin and Worthing, 1977) *

N° 38: 2,3,7,8-tetrachlorodibenzo-p-dioxin

Formula:	**$C_{12}H_4Cl_4O_2$**
CAS Registry Number:	1746-01-6
Molecular weight:	321.97
Aqueous solubility:	0.0000193 mg/l at 25 °C (selected by Shiu *et al.*, 1988)
	0.000317 mg/l at 25 °C (Schroy *et al.*, 1985) *
	0.0000193 mg/l (Marple *et al.*, 1986)
	0.00000791 mg/l (Adams and Blaine, 1986)
	0.000419 mg/l at 22.7 °C (Friesen *et al.*, 1990)
	0.000441 mg/l at 22.7 °C (Friesen *et al.*, 1990)
log P (octanol-water):	6.80 at 25 °C (R) (Shiu *et al.*, 1988) *
	7.14 (C) (Mackay *et al.*, 1985)
	6.15 (Schroy *et al.*, 1985)
	6.42 (D) (Sijm *et al.*, 1989)
	7.02 (I) (Burkhard and Kuehl, 1986)
	5.5 (I) (Kaiser, 1983)
Vapor pressure:	0.0000035 Pa at 25 °C (Rordorf, 1985)
	0.0000063 Pa at 25 °C (Rordorf, 1985)
	0.0000045 Pa at 25 °C (Rordorf, 1985) *
	0.000000099 Pa at 25 °C (Podoll *et al.*, 1986)
	0.000000461 Pa at 30.1 °C (Schroy *et al.*, 1985)
	0.0000183 Pa at 54.6 °C (Schroy *et al.*, 1985)
	0.0000497 Pa at 62 °C (Schroy *et al.*, 1985)
	0.000159 Pa at 71 °C (Schroy *et al.*, 1985)

N° 39: Toluene:

Formula:	**C_7H_8**
CAS Registry Number:	108-88-3
Molecular weight:	92.14
Aqueous solubility:	538 mg/l at room Temp. (25 +/- 1.5 °C) (McAuliffe, 1963)
	515 mg/l at room Temp. (25 +/- 1.5 °C) (McAuliffe, 1966)

Table 1 (continued)

	573 mg/l at 25 °C (Polak and Lu, 1973)
	627 mg/l at 25 °C (Bohon and Claussen, 1951)
	578.64 mg/l at 25 °C (Wasik *et al.*, 1983) *
	470 mg/l at 16 °C (Chiou *et al.*, 1977)
	580 mg/l at 25 °C (Keeley *et al.*, 1988)
	1548 mg/l at 25 °C (Banerjee *et al.*, 1980)
	479 mg/l at 21 °C (Chey and Calder, 1972)
	534.8 mg/l at 25 °C (Sutton and Calder, 1975)
	530 mg/l at 25 °C (Andrews and Keefer, 1949)
	578.64 mg/l at 25 °C (Tewari *et al.*, 1982)
	570 mg/l at 30 °C (Gross and Saylor, 1931)
log P (octanol-water):	2.21 at 23 °C (D) (Banerjee *et al.*, 1980)
	2.65 at 25 °C (D) (Wasik *et al.*, 1983) *
	2.65 at 25 °C (D) (Tewari *et al.*, 1982)
	2.65 at 25 °C (D) (Schantz and Martire, 1987)
	2.68 (D) (Nahum and Horvath, 1980)
	2.69 at 25 °C (D) (Hansch *et al.*, 1968)
	2.69 (Leo *et al.*, 1971)
	2.69 (C) (Chiou *et al.*, 1977)
	2.73 (Leo *et al.*, 1971)
	2.11 (Leo *et al.*, 1971)
	2.80 (Leo *et al.*, 1971)
	2.51 (I) (Mackay *et al.*, 1980)
	2.51 (I) (Eadsforth, 1986)
	3.06 (I) (Eadsforth, 1986)
	2.64 (I) (Schantz and Martire, 1987)
	2.76 (I) (Arbuckle, 1983)
	2.87 (I) (Arbuckle, 1983)
	2.88 (I) (Campbell and Luthy, 1985)
	2.94 (I) (Könemann *et al.*, 1979)
	2.73 (R) (Sangster, 1989)
	2.69 (Anonymous, 1988g)
	2.78 (I) (Burkhard *et al.*, 1985b)
	2.79 (I) (Burkhard *et al.*, 1985b)
	2.21 at 20 °C (D) (Veith *et al.*, 1980)
	2.99 (I) (Veith *et al.*, 1980)
	2.79 (I) (Veith *et al.*, 1980)
	2.66 (I) (Klopman and Iroff, 1981)
	2.70 (I) (Klopman and Iroff, 1981)
	2.63 (I) (Klopman and Iroff, 1981)
	2.46 (I) (Klopman *et al.*, 1985)
	2.42 (I) (Klopman *et al.*, 1985)
	3.00 (I) (De Kock and Lord, 1987)
	2.79 (I) (De Kock and Lord, 1987)
	2.89 (I) (Rapaport and Eisenreich, 1984)
	2.96 (I) (McDuffie, 1981)
	2.65 (I) (Harnisch *et al.*, 1983)
	2.77 (I) (Harnisch *et al.*, 1983)
	2.78 (I) (Hammers *et al.*, 1982)

Table 1 (continued)

	2.59 (I) (D'Amboise and Hanai, 1982)
	2.88 (I) (Eadsforth and Moser, 1983)
Vapor pressure:	3792 Pa at 25 °C (Zwolinski and Wilhoit, 1971) *
	3791 Pa at 25 °C (Hine and Mookerjee, 1975)
	3826 Pa at 25 °C (Anonymous, 1988g)
	3799 Pa at 25 °C (Sundaram and Leung, 1986)
	3795 Pa at 25 °C (Bohon and Claussen, 1951)

N° 40: Toxaphene (camphechlor)

Formula:	**$C_{10}H_{10}Cl_8$**
CAS Registry Number:	8001-35-2
Molecular weight:	413.81
Aqueous solubility:	0.74 mg/l at 25 °C (Weil *et al.*, 1974)
	0.5 mg/l (Paris *et al.*, 1977)
	0.5 mg/l at 25 °C (Anonymous, 1988d) *
	3 mg/l at 25 °C (Anonymous, 1988d)
	0.55 mg/l at 20 °C (Murphy *et al.*, 1987)
	0.5 mg/l at 20 °C (R) (Suntio *et al.*, 1988)
	0.4 mg/l (Kenaga, 1980a)
	3 mg/l at room Temp. (Martin and Worthing, 1977)
log P (octanol-water):	3.52 (Paris *et al.*, 1977)
	3.3 (R) (Suntio *et al.*, 1988)
	5.50 (C) (Garten and Trabalka, 1983)
	2.92 (Anonymous, 1988d)
	3.52 (Anonymous, 1988d) *
Vapor pressure:	22.66 - 53.32 Pa at 25 °C (Anonymous, 1988d)
	0.0005 Pa at 20 °C (R) (Suntio *et al.*, 1988) *
	26.66 - 53.32 Pa at 25 °C (Martin and Worthing, 1977)

N° 41: 2,4,6-trichlorobiphenyl

Formula:	**$C_{12}H_7Cl_3$**
CAS Registry Number:	35693-92-6
Molecular weight:	257.55
Aqueous solubility:	0.226 mg/l at 25 °C (Miller *et al.*, 1984) *
	0.252 mg/l at 25 °C (Dunnivant and Elzerman, 1988)
	0.0804 mg/l at 4 °C (Doucette and Andren, 1988)
	0.187 mg/l at 25 °C (Doucette and Andren, 1988)
	0.435 mg/l at 40 °C (Doucette and Andren, 1988)
log P (octanol-water):	5.47 at 25 °C (D) (Miller *et al.*, 1984) *
	5.50 (R) (Shiu and Mackay, 1986)
Vapor pressure:	0.0124 Pa at 25 °C (Burkhard *et al.*, 1985a) *

N° 42: 2,4,6-trichlorophenol

Formula:	**$C_6H_3Cl_3O$**
CAS Registry Number:	88-06-2
Molecular weight:	197.45
Aqueous solubility:	434 mg/l at 25 °C (Jones, 1981) *
log P (octanol-water):	3.06 (Leo *et al.*, 1971)
	3.69 (Leo *et al.*, 1971)

Table 1 (continued)

	3.64 at 20 °C (I) (Xie and Dyrssen, 1984)
	3.65 at 20 °C (I) (Xie and Dyrssen, 1984)
	3.66 at 20 °C (I) (Xie and Dyrssen, 1984)
	3.75 (D) (Xie *et al.*, 1984) *
	3.69 (I) (Xie *et al.*, 1984)
	3.77 (I) (Xie *et al.*, 1984)
	3.73 (I) (Xie *et al.*, 1984)
	3.29 (I) (Chin *et al.*, 1986)
Vapor pressure:	3.26 Pa at 25 °C (Bidleman and Renberg, 1985) *

3. Structure-environmental fate relationships

Correspondence factor analysis of the data matrix (6 x 42) shows that the first two factorial axes explain 100% of the total inertia (F1, F2 accounting for 54.1% and 45.9% respectively). The graphical display of the variables (figure 1) clearly reveals that the six compartments are distributed into three clusters: AIR, WATER, and SOIL-SEDIMENT-SUSPENDED SEDIMENT-BIOTA. Air lies in the upper left corner, water on the right hand side, and the third cluster in the lower left corner of the factorial plane F1F2. The opposition between these three clusters seemed a priori logical and has been stressed in recent publications (Devillers *et al.* 1989a, Devillers and Karcher, 1990a). The clustering of soil, sediment, suspended sediment, and biota is due to the influence of the partition coefficient (log P).

The graphical display of the objects (figure 2) shows that the chemicals are distributed between the three above clusters. Examination of the chemical structures of these organic pollutants (figure 2) allows the establishment of structure-distribution relationships. Aromatic compounds containing only carbon and hydrogen atoms are distributed relatively to their size from air to the soil cluster. Thus, benzene (compound number 5), 1,3-dimethyl benzene (compound 19), ethylbenzene (compound 21), and toluene (compound 39) whose formulae are C_6H_6, C_8H_{10}, C_8H_{10} and, C_7H_8, respectively are located at the top of figure 2 (i.e.; in the air compartment). Naphthalene (compound 31, $C_{10}H_8$) is located just below these compounds with C_6 to C_8. Further down, are displayed acenaphthene (compound 1) and biphenyl (compound 6) which present an increased number of carbon atoms (i.e.; $C_{12}H_{10}$). Fluorene (compound 23, $C_{13}H_{10}$) lies midway between air and soil cluster. Then, below F1 axis are encountered phenanthrene (compound 34) and anthracene (compound 3) with their same formula: $C_{14}H_{10}$. Fluoranthene (compound 22) and pyrene (compound 36) of formula $C_{16}H_{10}$ lie further down. Benz(a)anthracene (compound 4, $C_{18}H_{12}$), the biggest PAH of the data set is located at the bottom of figure 2 (i.e.; in the soil cluster). In conclusion, the theoretical environmental distribution of PAHs and related compounds between air and soil cluster can be plotted on a scale based on the number of carbon atoms (figure 2). However, we note that the structural features also play a key role in the environmental distribution of chemicals. Biphenyl (compound 6) and acenaphthene (compound 1), with the same formula (i.e.; $C_{12}H_{10}$), and a different molecular graph are not superimposed on figure 2. A similar remark can be made for anthracene (compound 3) and phenanthrene (compound 34).

The environmental distribution of PCBs is governed by their degree of substitution, allowing to draw a scale based on the number of chlorine atoms (figure 2). Thus, biphenyl

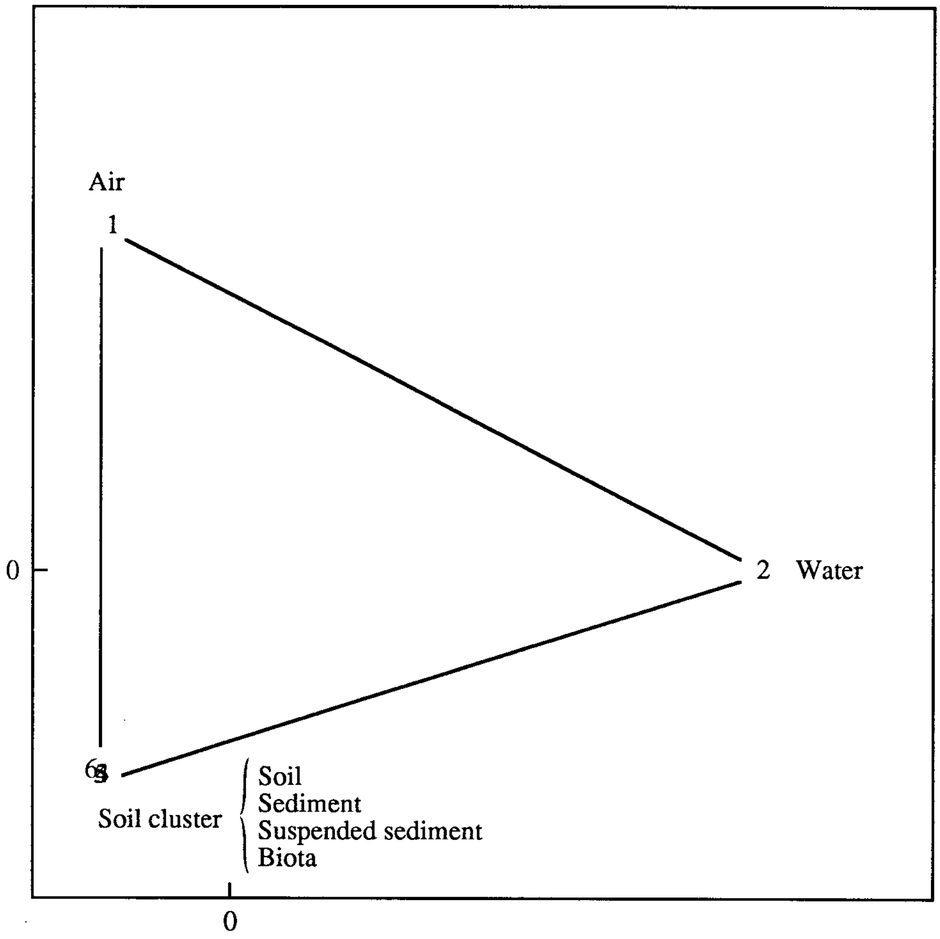


Figure 1: First two factors map for the 6 compartments of the CFA performed on the 42 chemicals under study. The triangular shape of the figure comes from the fact that the structure of the data set is mainly three-dimensional. Thus, the position of each point inside this triangle will be directly given by the distribution of the chemicals between the three vertices (see figure 2).

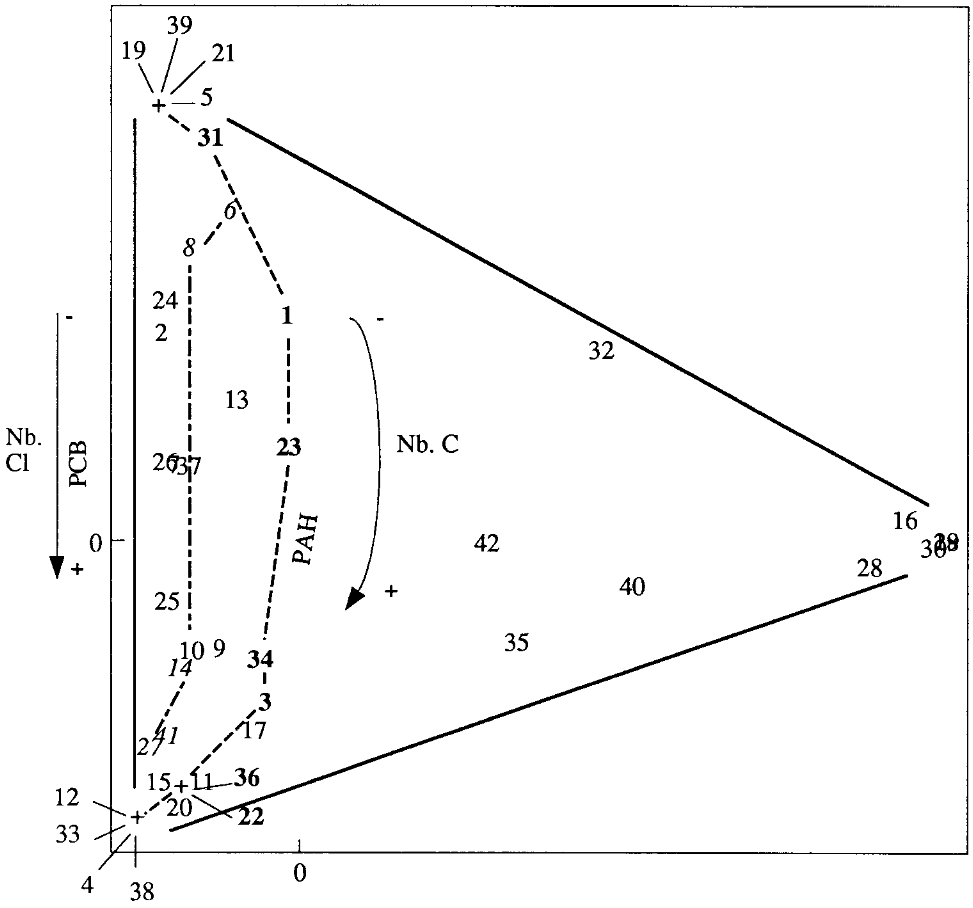


Figure 2: First two factors map of the CFA for the 42 chemicals under study.

(compound 6), 2-chlorobiphenyl (compound 8), 2,5-dichlorobiphenyl (compound 14), 2,4,6-trichlorobiphenyl (compound 41), and 2,2',4,4',6,6'-hexachlorobiphenyl (compound 27), in which the number of chlorine atoms rises from 0 to 6, shift down from air to soil cluster . The same remark can be made for dioxin derivatives. Thus, dibenzo-p-dioxin (compound 13) is located nearly half-way between air and soil cluster. Compound 9 (1-chlorodibenzo-p-dioxin) and 2-chlorodibenzo-p-dioxin (compound 10) lie below. Further down, 2,7-dichlorodibenzo-p-dioxin (compound 15) is found. The most substituted dioxins (i.e.; 2,3,7,8-tetrachlorodibenzo-p-dioxin (compound 38) and octachlorodibenzo-p-dioxin (compound 33)) are located at the bottom of figure 2. Besides these direct structure-distribution relationships, it could be interesting to stress the basic physicochemical properties governing them. To reach this goal, the values of the parameters used in the calculations of the fugacity model level I, have been projected onto figure 2 by means of squares (positive values) and circles (negative values) proportional to their magnitude (figure 3a-d). For graphical conveniences, all the solubility and vapor pressure data were expressed as their decimal logarithm like the n-octanol water partition coefficient. In order to know if the distribution is due to one or more parameters at a time, we also projected the Henry's constant expressed as its logarithm (figure 3e). Lastly, a collection of graphs has been made from the number of each chemical element (i. e.; C, H Cl, N, O, P, S) included in the studied molecules (figure 4a-g). Inspection of figure 3a allows to point out that the molecular weight is an underlying feature of the observed structure-distribution relationships as it can be seen that low molecular weight compounds (small squares) are preferentially found at the top of figure 3a (i.e.; in air). This explains the gradual shift of PAHs from air to soil cluster. There is also an obvious relation between the aqueous solubility and the chemical distribution (figure 3b). Compounds with very low solubilities (circles) are only located in the soil cluster while those with a high solubility can be found either in water or air compartments. Therefore, this property is not sufficient to discriminate the whole set of chemicals. Figure 3c shows that organic pollutants with high log P values are always located in the soil cluster and never in water and air compartments. Compounds with very high vapor pressure values (large squares) are only located in the air compartment, lower data distributing either to water or soil clusters. From the above results, it appears obvious that one physicochemical property cannot alone explain the environmental distribution of an organic chemical. Observation of figure 3e confirms this hypothesis. Indeed, the Henry's law constant obtained from water solubility and vapor pressure data shows a strong discriminating power. Figure 4a reveals a general relationship between the number of carbon atoms contained in the molecules and their environmental distribution, since the little squares (i.e.; compounds with few carbon atoms) are not located in the soil cluster. This figure is quite similar to figure 3a. This is not surprising due to the key role of the carbon atoms in our set of molecules. At the opposite, it seems obvious that the number of hydrogen contained in molecules (figure 4b) is not discriminating. Figure 4c shows that chemicals without chlorine atom can be found in the three main clusters. However, it appears that there is a strong correlation between the number of chlorine atoms contained in molecules and their environmental distribution. For a same chemical family, compounds with few chlorine atoms are preferentially located in the air or water compartments while an increasing of the number of this element results in the shift down to the soil cluster. Figure 4d reveals a strong influence of the presence of nitrogen atoms in the molecules on their environmental distribution. Indeed, nitrogenous molecules of our data set are mainly found in the water compartment. The two chemicals which transgress this statement are chlorpyrifos (compound 11) and nitrobenzene (compound 32). The location of chlorpyrifos (i.e.; soil compartment) may be explained by the fact that this compound has its nitrogen atom contained in an aromatic ring (pyridine ring), and not in an amine, amide or nitro functional group. Therefore, its influence is

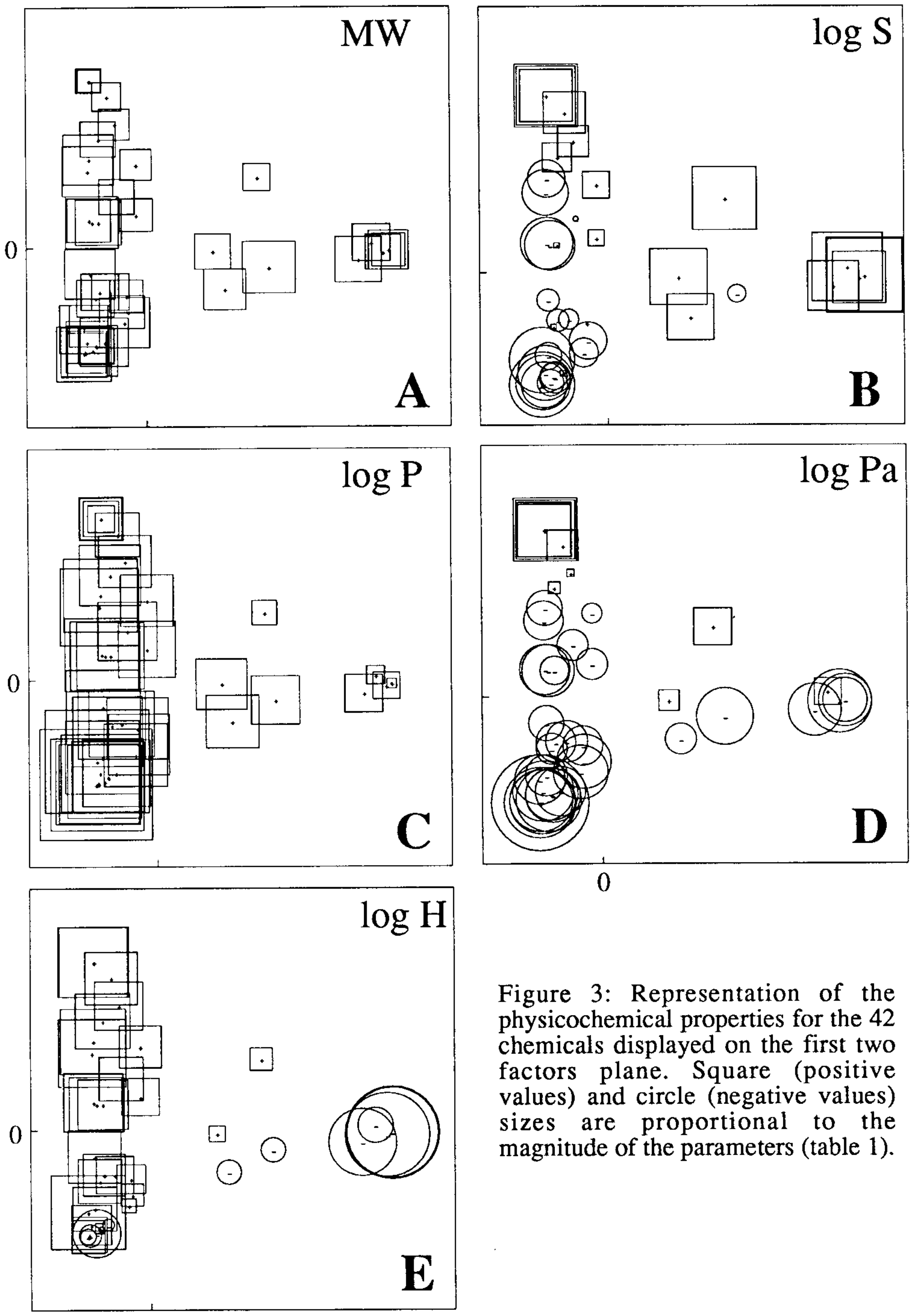


Figure 3: Representation of the physicochemical properties for the 42 chemicals displayed on the first two factors plane. Square (positive values) and circle (negative values) sizes are proportional to the magnitude of the parameters (table 1).

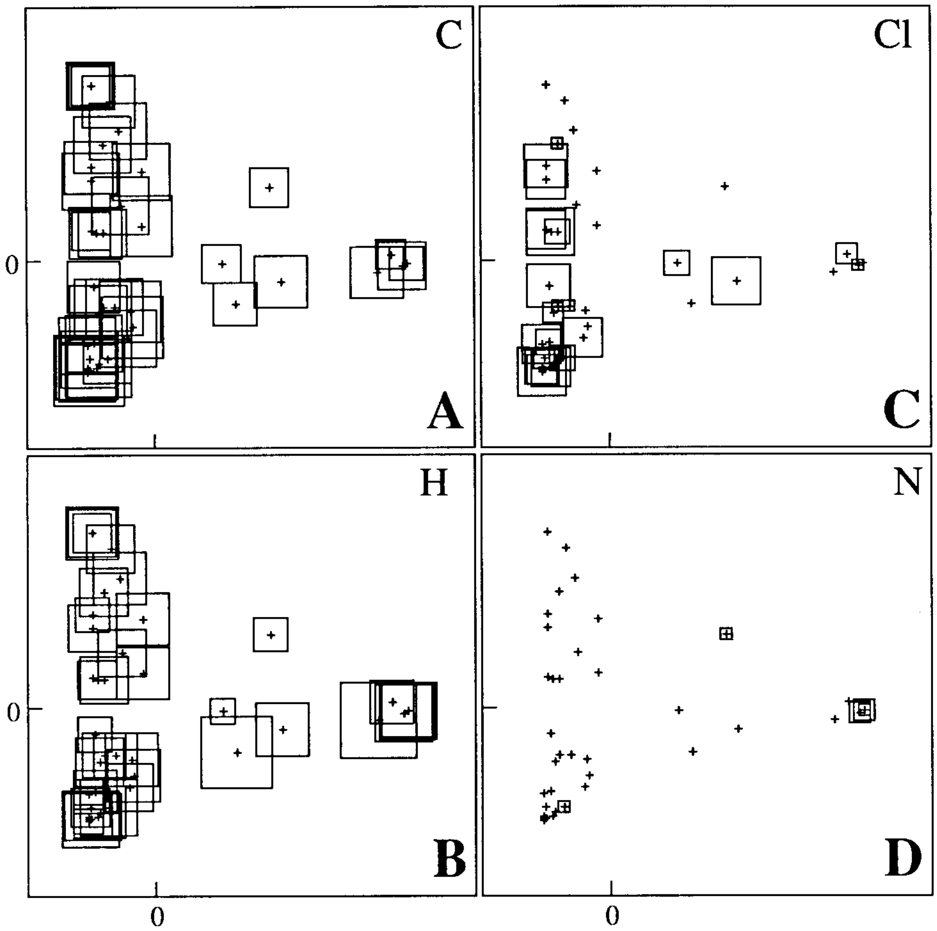


Figure 4 (A to D): Representation of the number of carbon (A), hydrogen (B), chlorine (C), and nitrogen (D) atoms for the 42 chemicals displayed on the first two factors plane. Square sizes are proportional to the number of atoms.

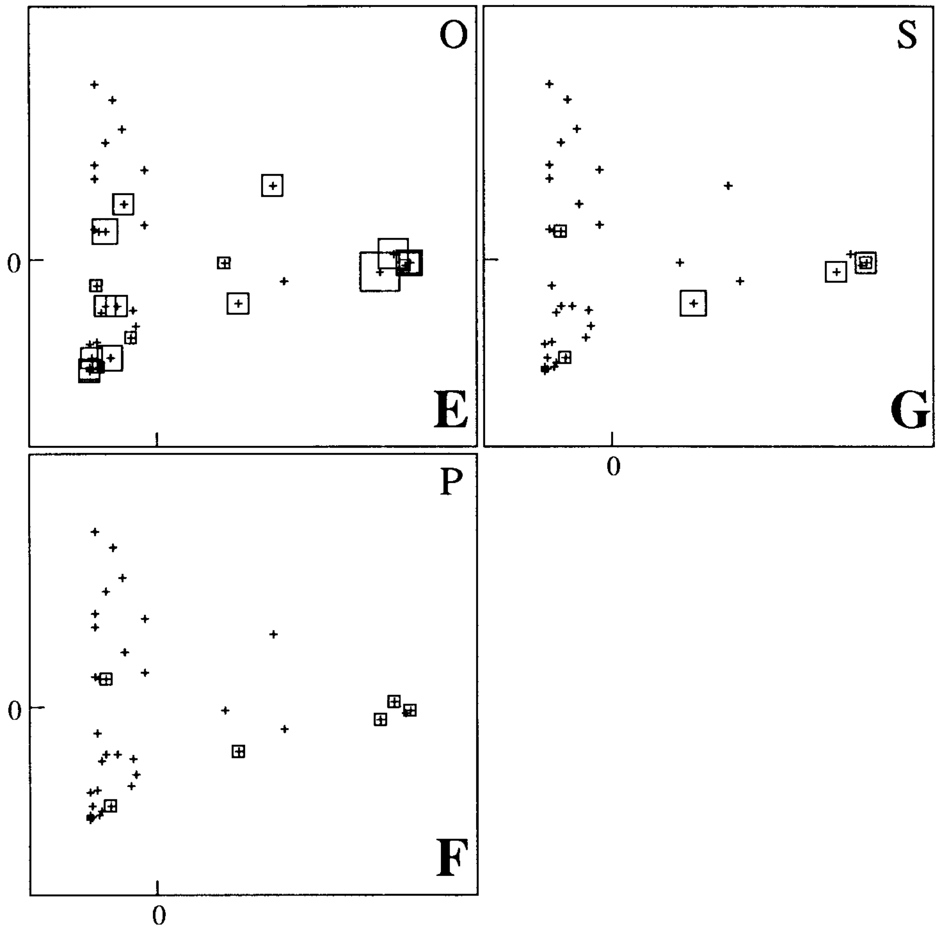


Figure 4 (E to G): Representation of the number of oxygen (E), phosphorus (F), and sulfur (G) atoms for the 42 chemicals displayed on the first two factors plane. Square sizes are proportional to the number of atoms.

quite different. The location of nitrobenzene (i.e.: between air and water compartments) when compared to this of benzene (i.e.; air compartment) is explained by the fact that these compounds are both quite soluble but nitrobenzene exhibits a smaller vapor pressure value pulling it down to water. Its location compared to those of the other chemicals of our data set containing nitrogen atoms, might be explained by the fact that it is the only compound with a NO_2 functional group. Inspection of figure 4e stresses the effect of oxygen atom on the environmental fate of chemicals, since such molecules are found in water and soil cluster. Chemicals with phosphorus atoms (figure 4f) as those which contain oxygen atoms do not distribute into the air compartment. Finally, the same remark can be made for chemicals which contain sulfur atoms (figure 4g). Among the 42 chemicals under study, those with phosphorus and/or sulfur atoms are pesticides. Therefore, it is not surprising that they are located in the water and/or soil cluster (figure 4f-g).

The above graphical and statistical analyses clearly demonstrate that it is possible to establish structure-distribution relationships from the results of the fugacity model level I.

4. Influence of the variability in the input data

Our results clearly demonstrate that the environmental distribution of a chemical highly depends on its basic physicochemical properties. Therefore, great care must be taken in the selection of these data for hazard ranking. As it can be noticed in table 1, different degrees of variability are encountered for the physicochemical properties of organic compounds. It is obvious that this variability must influence the outputs obtained with the fugacity model level I.

Multivariate analyses can be used to estimate how important is the effect of the variability. However, in a first step, to be coherent, it was necessary to take into account the following constraints in the data selection:

- aqueous solubility and vapor pressure values have to be experimentally measured in a 20 to 25°C range. This choice is justified by the facts that first, the number of available data measured at 20 or 25°C is rather scarce; second, a low variability is expected in this range; third, this interval of temperatures is the one which is generally considered in such studies (Rippen *et al.*, 1984; Cohen and Ryan, 1985; Gaggi *et al.*, 1985; Calamari and Bacci, 1987; Vighi *et al.*, 1987; Clark *et al.*, 1988); last, authors often give an estimated temperature like: room temperature (Robeck *et al.*, 1965; Martin and Worthing, 1977), or 25+/-1.5°C (McAuliffe, 1963; 1966; Reinert, 1987).
- for partition coefficient, we considered data measured by direct and indirect methods since both are widely used in QSAR studies (Saarikoski and Viluksela, 1982; Benoit-Guyod *et al.*, 1984; Broderius and Kahl, 1985; Call *et al.*, 1985; Vighi and Calamari, 1985; Zaroogian *et al.*, 1985; Schultz *et al.*, 1986; Yoshioka *et al.*, 1986a, b; Babich and Borenfreund, 1987; Abernethy *et al.*, 1988; Donkin *et al.*, 1989)

Calculation of all the possible environmental distributions (i.e.; for each combination of aqueous solubility, vapor pressure, and partition coefficient values) was achieved by means of the statistical module of the CFMP software (Devillers and Karcher, 1990b). For the computation of these data, we entered a value only once for a given chemical so as to prevent from redundancy. This resulted in 10,301 different combinations (excluding the 42 previously calculated distributions which are displayed in figure 2). These results are exploited by projecting all the resulting distributions for a chemical as supplementary objects on the factorial plane of the chemicals (figure 2). A collection of 42 maps was obtained (figures 5.1 to 5.42, the second number corresponding to the chemical).

From these maps, numerous observations can be made. First, it is interesting to note that the scattering of the supplementary points on the plane F1F2 is not the same for all the

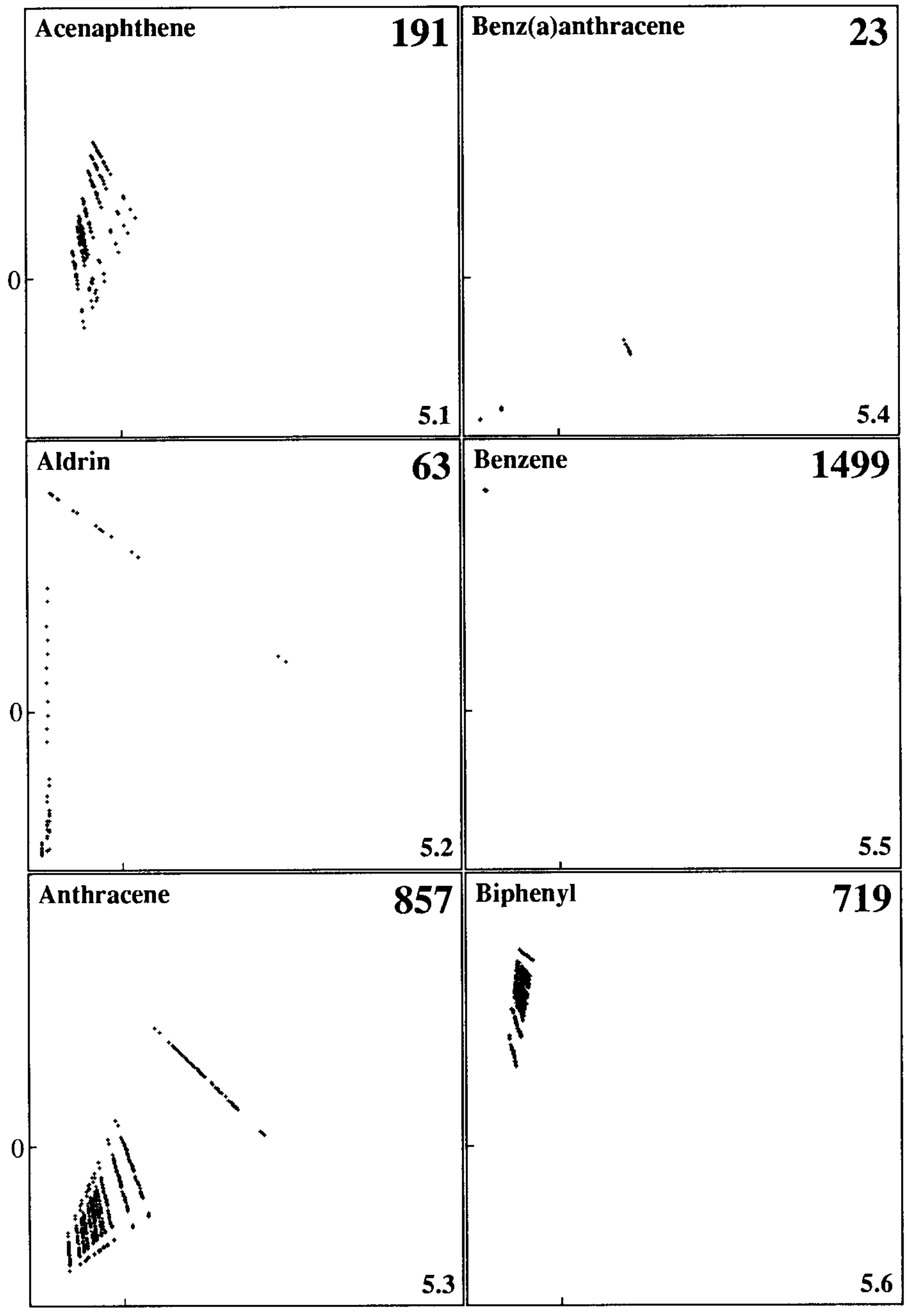
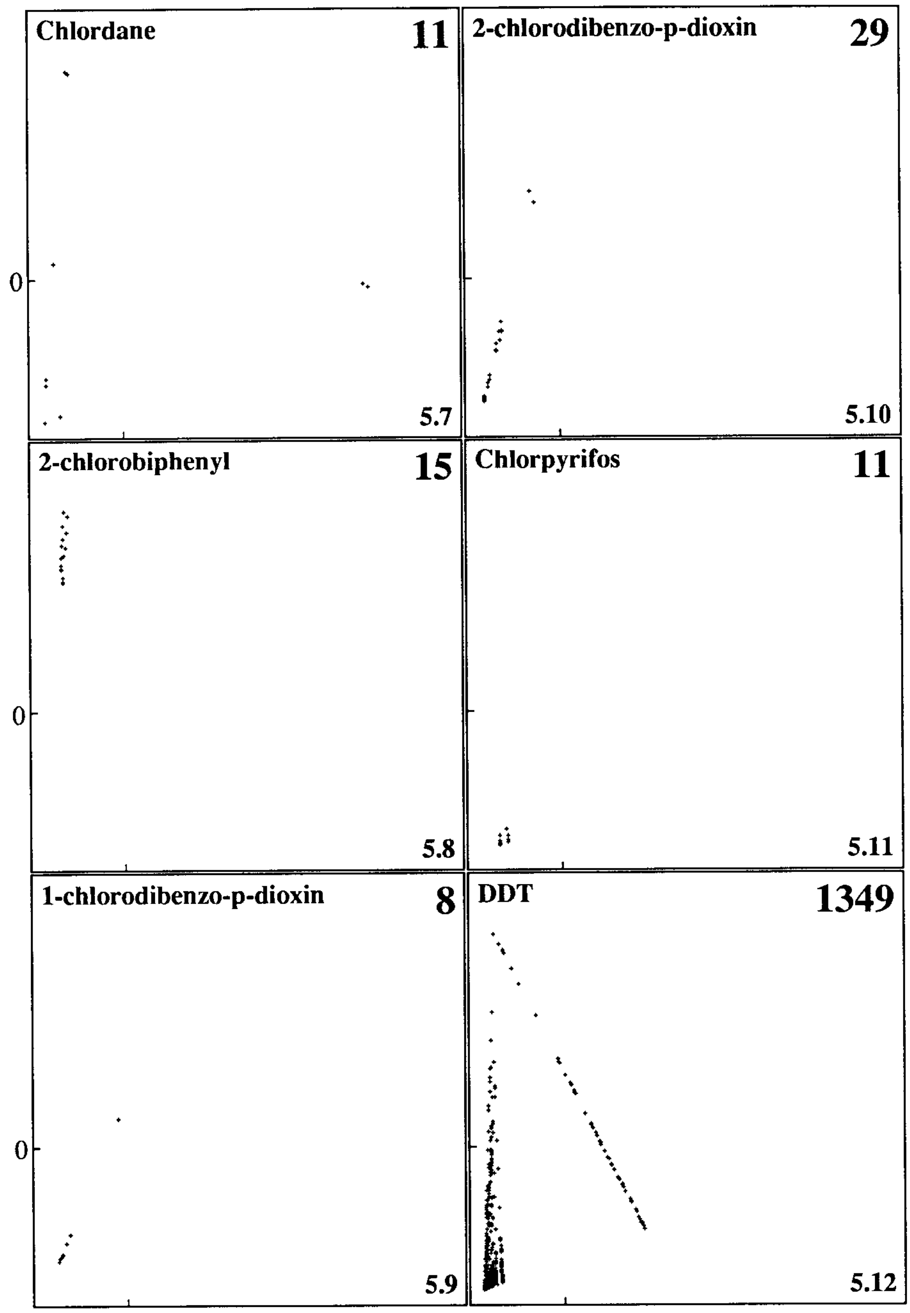


Figure 5 (5.1 to 5.6): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.



Chlordane

2-chlorodibenzo-p-dioxin

2-chlorobiphenyl

Chlorpyrifos

1-chlorodibenzo-p-dioxin

DDT

Figure 5 (5.7 to 5.12): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

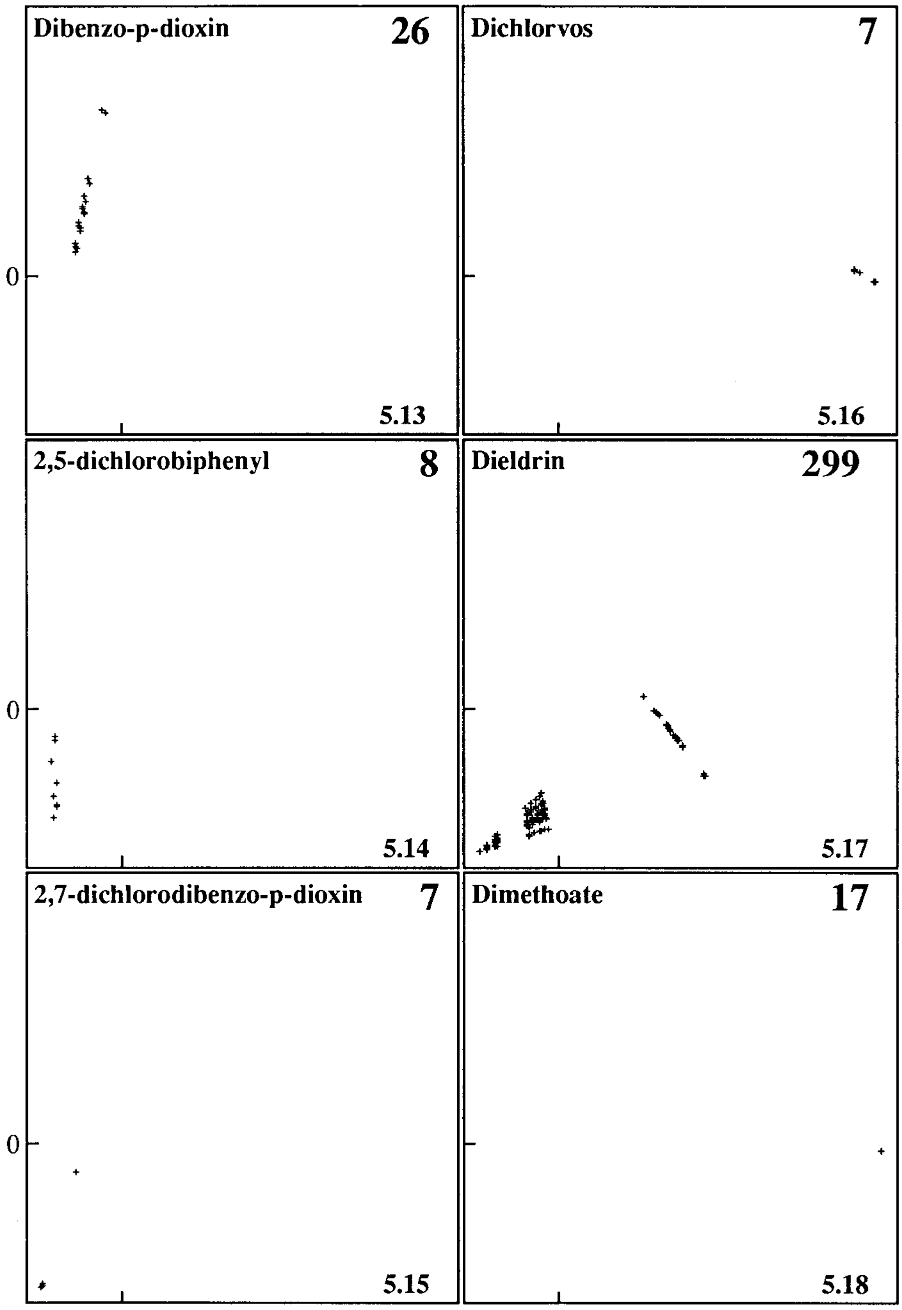


Figure 5 (5.13 to 5.18): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

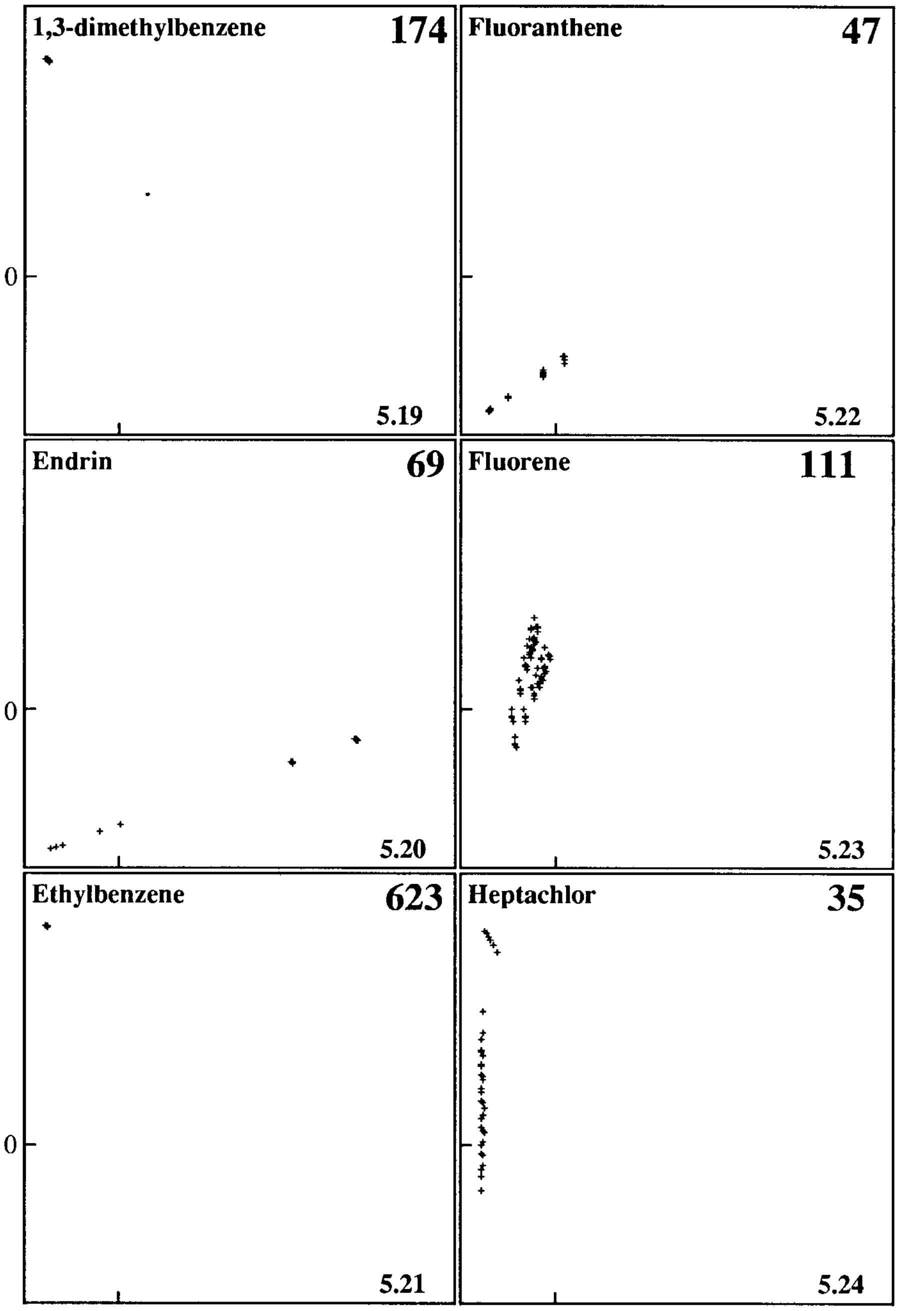


Figure 5 (5.19 to 5.24): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

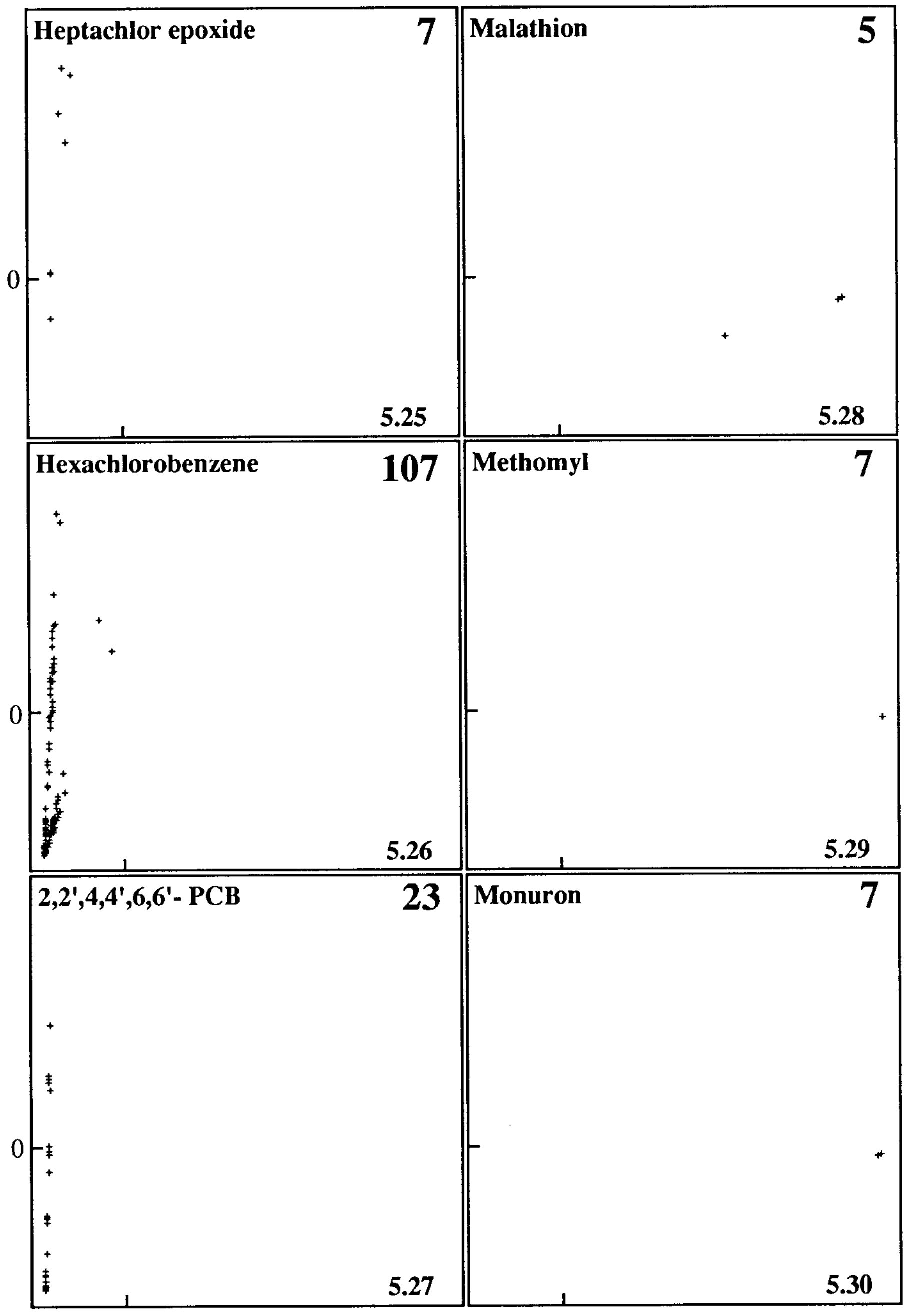


Figure 5 (5.25 to 5.30): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

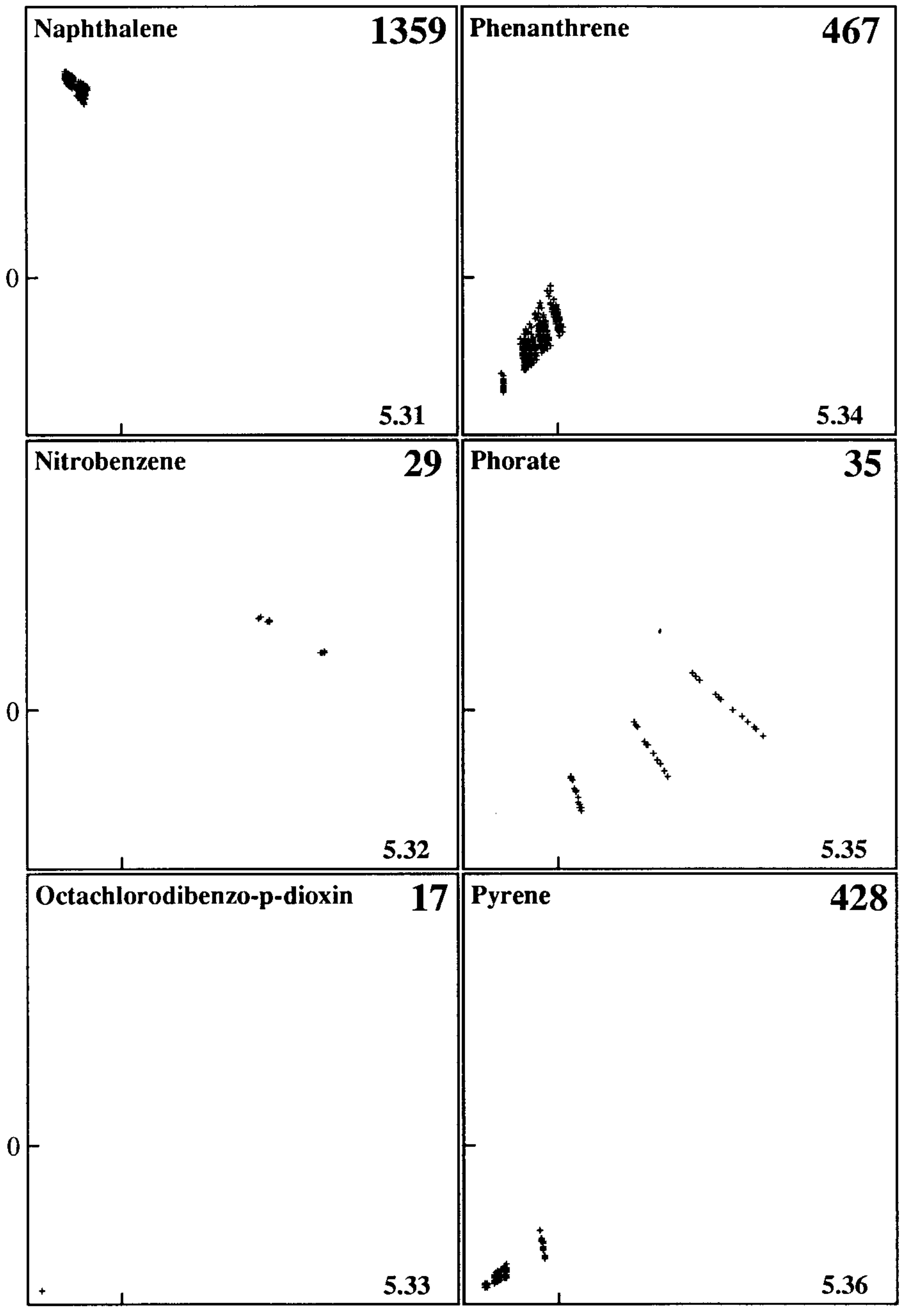


Figure 5 (5.31 to 5.36): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

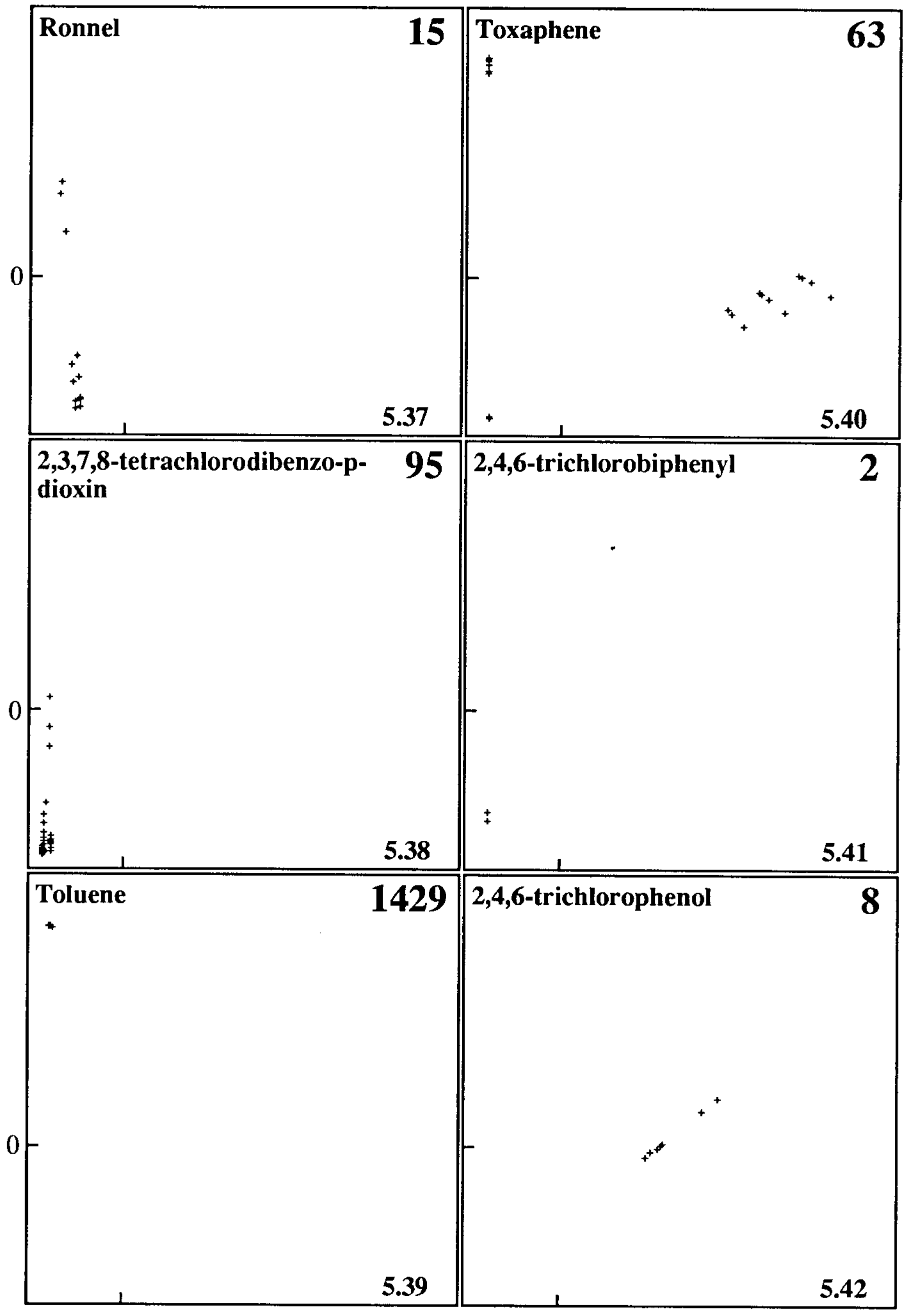


Figure 5 (5.37 to 5.42): Projection of the environmental distributions obtained from the different combinations of the selected physicochemical data in table 1.

chemicals under study. Thus, the 1499 supplementary points of benzene (figure 5.5), 17 points of dimethoate (figure 5.18), 174 points of 1,3-dimethylbenzene (figure 5.19), 623 points of ethylbenzene (figure 5.21), or 1429 points of toluene (figure 5.39) are superimposed. At the opposite, the scattering of the supplementary points for aldrin (figure 5.2; 63 points), anthracene (figure 5.3; 857 points); chlordane (figure 5.7; 11 points), DDT (figure 5.12; 1349 points), endrin (figure 5.20; 69 points), heptachlor (figure 5.24; 35 points), or hexachlorobenzene (figure 5.26; 107 points) is very large. Among this last category, notice that the supplementary points of aldrin (figure 5.2), chlordane (figure 5.7), and DDT (figure 5.12) can be included in a triangle with a small base. From the above graphical observations it is obvious that the scattering of the different outputs is linked to the structure of the molecules (e.g.; difference between pesticides, PAH, and alkyl benzenes). The practical applications of these results deal with hazard assessment. Indeed, the map obtained with benzene (figure 5.5), ethylbenzene (figure 5.21) or toluene (figure 5.39) reveals that it is not useful to try to select accurate input data among all the different values available in the literature (table 1) since in all cases the outputs are the same (i.e.; the pollutants stay in their main compartment). Conversely, great care must be taken in the selection of the inputs for pesticides, PAH, and related compounds since the outputs can be very different. Thus, for example, we can note that from the different inputs available for chlordane (table 1) we can find that this pesticide presents a great affinity for the air, water, or soil cluster (figure 5.7).

We then attempted to explain the different shapes of the clouds (figures 5.1 to 5.42). For this purpose, the physicochemical properties (i.e.; aqueous solubility, partition coefficient, and vapor pressure) were projected onto each point of these clouds by means of squares proportional to their values. Figures 6 to 10 correspond to the chemicals for which the most significant results were obtained. The triangular shape noticed for aldrin (figures 5.2 and 6) related to its potential affinity for air, water, or soil cluster and which depends on the combinations of the input data, is the result of different phenomena. The low values of log P are always found in air and water compartments, while large are necessarily in the soil cluster. This induces that the variability in the calculation of the environmental distributions of aldrin is not influenced by its aqueous solubility. Low and large vapor pressure values can be found in both air and soil cluster, while water only contains low values (figure 6). Figure 7 (anthracene) shows that there exist an aqueous solubility gradient running to the water compartment and a log P gradient running to the soil cluster. There is no gradient for vapor pressure. The log P gradient reveals that one of the values is atypical. Confirmation of this observation can be made from inspection of table 1. Indeed, all the partition coefficient values are ranged between 4.2 and 4.95 except one from Veith *et al.* (1979a) equal to 3.45. Therefore, this type of approach can be used to stress atypical data. A log P gradient is also observable for endrin (figure 8) running in the same direction (i.e.; from water to soil cluster) as the one observed for anthracene (figure 7). There is also no vapor pressure gradient. However, the aqueous solubility gradient is not observable any more.This must be attributed to the fact that endrin does not exhibit an appreciable variability about aqueous solubility values while the partition coefficients show a wide one. Results obtained for phorate (figure 9) are similar to those obtained for anthracene (figure 7) with only two gradients for aqueous solubility and log P values. The triangular shape observed for toxaphene (Figures 5.40 and 10) indicating its potential affinity for air, water, or soil cluster (related to the combinations of selected values for calculating the environmental distribution of toxaphene) arises from phenomena different from those observed for the previous selected compounds. Compared to the above figures, gradients are no longer observable neither for aqueous solubility nor for log P values (figure 10). We can suppose that these are hidden by the large effect of vapor pressure which shows a very wide variability (table 1). The very low value is found in water and soil cluster while

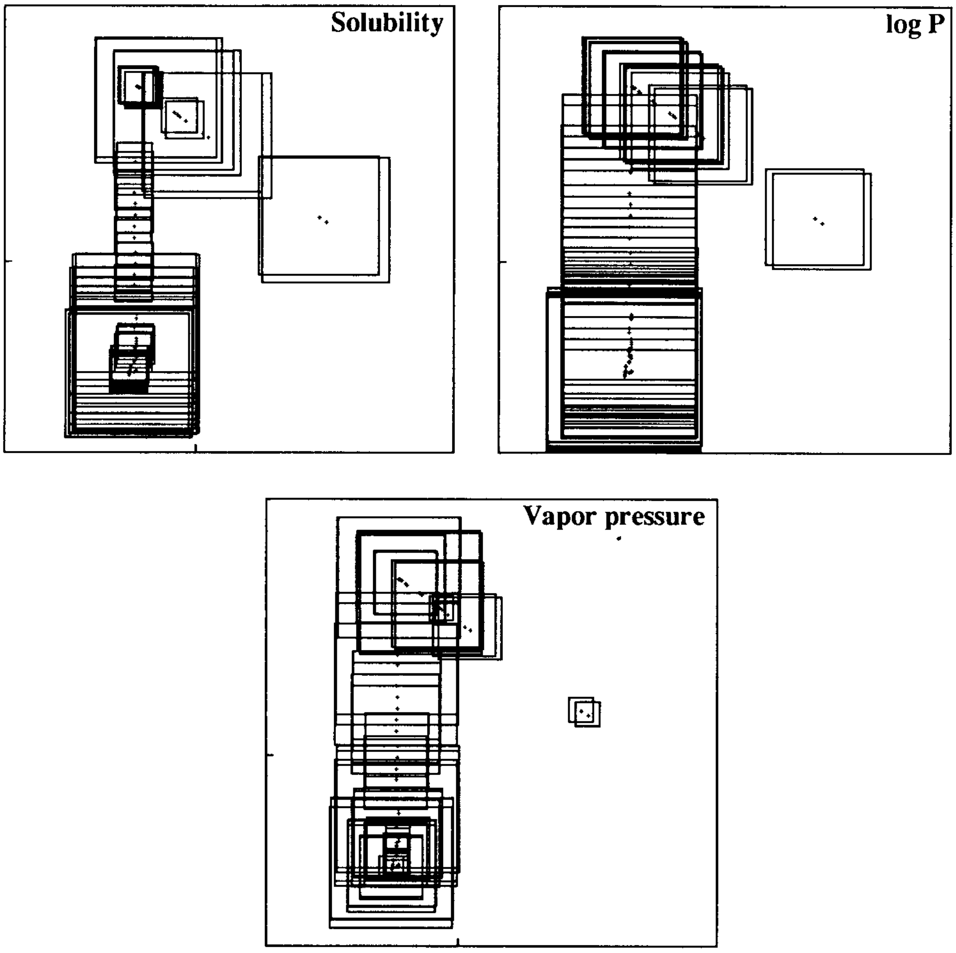


Figure 6: Representation of the three basic physicochemical properties for the 63 additional points of aldrin (square sizes are proportional to the values in table 1).

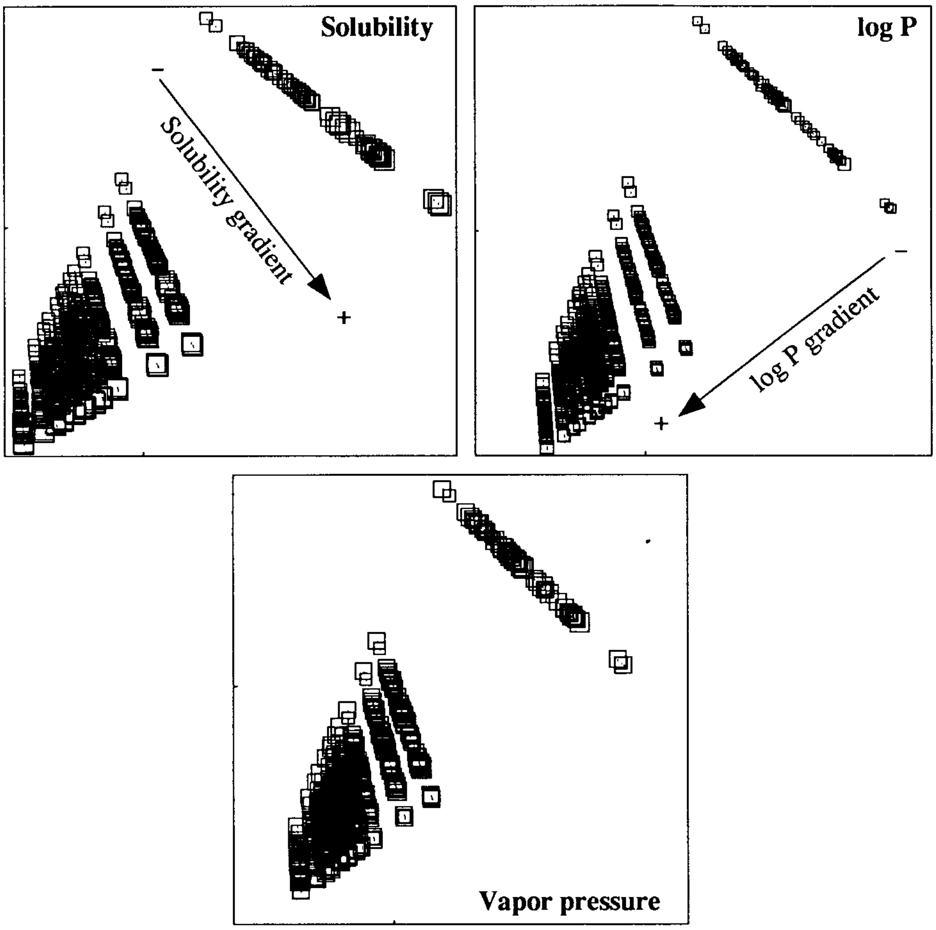


Figure 7: Representation of the three basic physicochemical properties for the 857 additional points of anthracene (square sizes are proportional to the values in table 1).

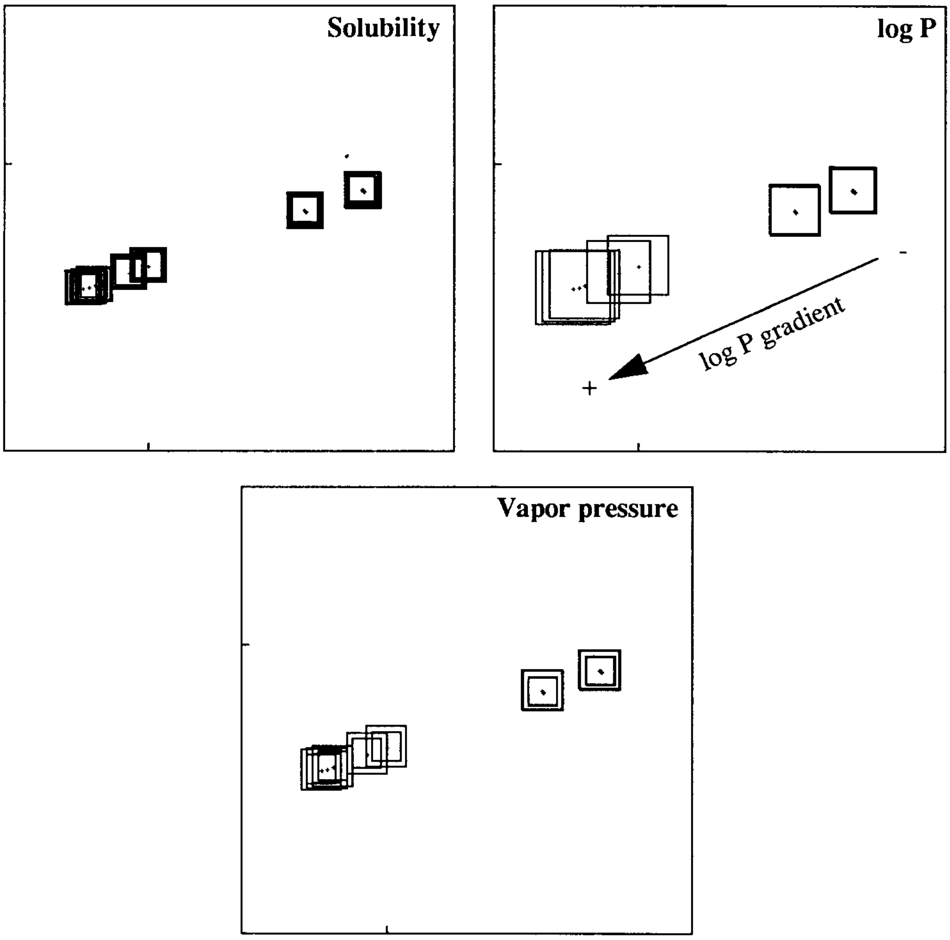


Figure 8: Representation of the three basic physicochemical properties for the 69 additional points of endrin (square sizes are proportional to the values in table 1).

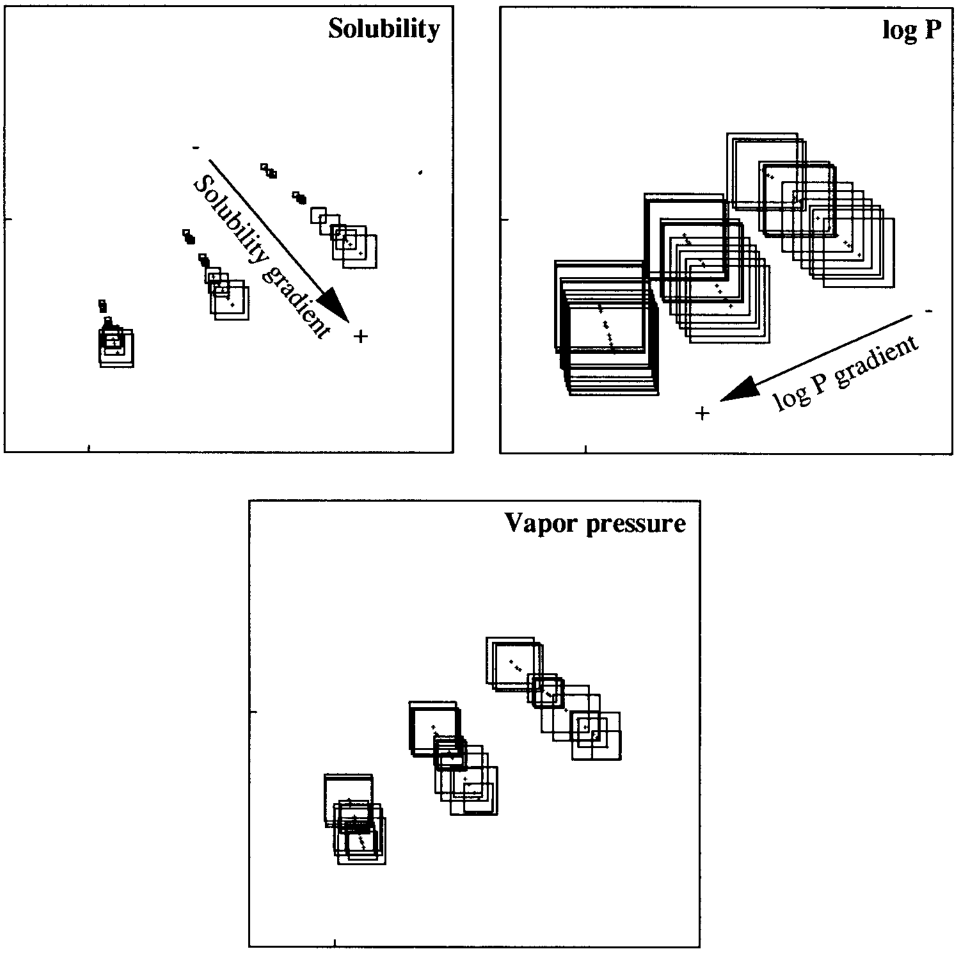


Figure 9: Representation of the three basic physicochemical properties for the 35 additional points of phorate (square sizes are proportional to the values in table 1).

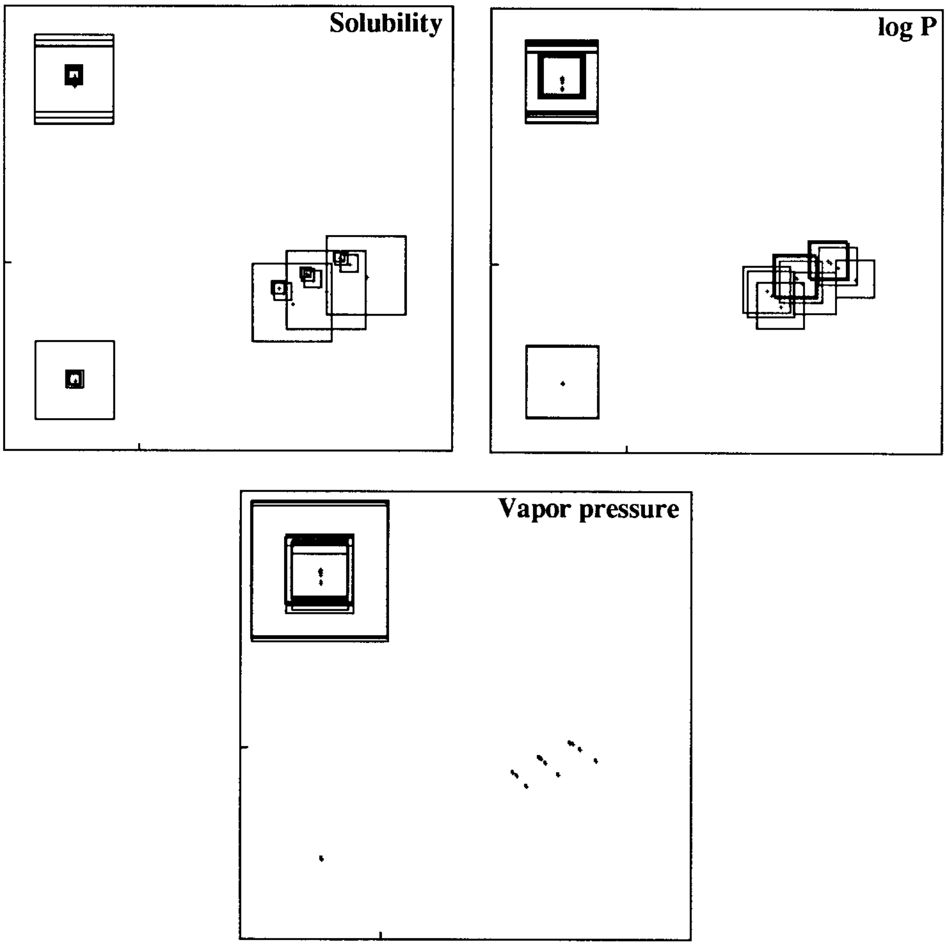


Figure 10: Representation of the three basic physicochemical properties for the 63 additional points of toxaphene (square sizes are proportional to the values in table 1).

large values are found in the air compartment. Figure 10 also reveals the usefulness of our graphical approach for stressing atypical data in the calculation of the distribution of the chemicals.

5. Conclusion

From the results of fugacity model level I, it has been demonstrated that it was possible to relate the environmental distribution of organic pollutants to their structures. The use of multivariate analyses especially when coupled to efficient graphical tools appears to be quite valuable for establishing such relationships. Projection on the factorial maps of the selected values for aqueous solubility, log P, and vapor pressure allows to find a physicochemical meaning to these relationships. Thus, the key role of log P was pointed out especially when values are quite high. This underlies the usefulness of critical reviews for partition coefficients (Eastcott *et al.*, 1988; Shiu *et al.*, 1988; Suntio *et al.*, 1988; Sangster, 1989), and the necessity of finding reliable methods of estimation. The results also reveal the combined importance of aqueous solubility and vapor pressure. This confirms the usefulness of the Henry's law constant for environmental fate models, especially when data are secured from experiments.

Since physicochemical data found in the literature are numerous and an appreciable variability is observed, it is obvious that this may influence the results obtained with fugacity model level I and induce variability. Our results underline the usefulness of multivariate analyses and graphical tools to estimate how important is this variability. The graphical maps reveal that the organic compounds under study give specific shapes of clouds which are related to the scattering of the outputs. Furthermore, each shape seems to be related to a chemical family (e.g.; pesticides, PAH). In some cases, a sole point is observed while some results cover the whole map meaning that the environmental distribution of the considered chemical is totally different according to the data selected. From a practical point of view, for the compounds giving a sole visible point for all the combinations of the input data, any value can be chosen from all the available data. At the opposite, the selection of data becomes very important for compounds which show a wide scattering. Unfortunately, these compounds are mainly the most hazardous for the environment. Projecting the values of the physicochemical properties onto each point of the clouds allows to stress their large influence on the environmental distribution of organic chemicals and especially the key role of log P.

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