Appendix C Substance-dependent data

In this Appendix, substance-dependent data are compiled to the extent that these are not provided in the main text. Data presented are those needed for the environmental fate (section C.1) and exposure assessment (C.2). Additionally, monitoring data are given in section C.3. While substance-dependent data involved in the impact assessment step of the Impact Pathway Approach have been fully given in the main text (cf. section 7.3), it shall be noted that substance-dependent valuation is not foreseen to be performed. This is due to the circumstance that results at the impact level may be aggregated according to the health endpoint such as DALYs (cf. section 7.3). As a result, there is for instance no section on monetary valuation in this Appendix.

C.1 Substance properties influencing the environmental fate

In the context of multimedia models, it is assumed that there is thermodynamic equilibrium within compartments. This means that substances partition between different phases of a compartment according to their ideal partitioning coefficients. Partitioning can occur between the solid and aqueous phase ('solid-water partitioning coefficients'), the gas and solid phase ('air-solid partitioning coefficient') as well as the gas and aqueous phase ('air-water partitioning coefficient'). Although it is tried in this documentation to use 'air', 'soil' and 'water' only for the air, soil and water compartment(s), respectively and not for phases, these terms are used here nevertheless as the notions 'solid-water partitioning coefficient' as well as the 'air-water partitioning coefficient' are commonly used.

C.1.1 Solid-water partitioning coefficient

In order to determine the solid-water partitioning coefficient, there are different approaches for different substances.

Lipophilic, non-dissociating organic substances

For lipophilic, non-dissociating substances, it is most common to base the solid-water partition coefficient on the octanol-water partition coefficient (K_{ow}). Usually first an organic carbon-water partition coefficient (K_{oc}) is derived (e.g., Brandes et al., 1996; Seth et al., 1999; McKone and Bennett, 2003). However, there is evidence that the goodness of the correlation between these two parameters is to be questioned (e.g., Seth et al., 1999; Baker et al., 2000, 2001). Seth et al. (1999) have shown that the usually good correlation between these two coefficients basically stems from an autocorrelation of the activity coefficient of the dissolved chemical fraction. Due to differing activity coefficients in the octanol phase and the organic carbon phase, a single correlation for all organic chemical classes is likely to be less accurate than class-specific models. This is supported by the observation that lipophilic organic chemicals although showing similar K_{ow} values have significantly different K_{oc} values (Chiou et al., 1998). Thus, Seth et al. (1999) recommend to use the following relationship:

$$K_{oc} = 0.00035 \cdot K_{ow} \tag{C-1}$$

where

0.00035 : empirical factor, conversion of theoretical unit from l per kg to m^3 per kg performed

K_{oc} : organic carbon-water partitioning coefficient [kg/kg C_{org} per kg/m^3_{water}]

K_{ow} : n-octanol water partitioning coefficient [kg/$m^3_{octanol}$ per kg/m^3_{water}].

Note that this is the partitioning coefficient between the organic carbon and the aqueous phase. In order to arrive at the overall partitioning coefficient between the aqueous and the (total) solid phase and assuming that the amount of chemical in the non-organic-carbon solid phase is zero, the solid-water partitioning coefficient is calculated by multiplying the K_{oc} value by the organic carbon content of the compartment:

$$K_{sw} = fr\_w_{\text{organic carbon/solid phase}} \cdot K_{oc} = 0.00035 \cdot fr\_w_{\text{organic carbon/solid phase}} \cdot K_{ow} \tag{C-2}$$

where

0.00035 : empirical factor, conversion of theoretical unit from l per kg to m^3 per kg performed fr_w : mass fraction of organic carbon in solid phase [kg C_{org} per $kg_{solid\ phase}$] (defined as described in section B.5)

K_{oc} : organic carbon-water partitioning coefficient [kg/kg C_{org} per kg/$m^3{}_{water}$]

K_{ow} : n-octanol water partitioning coefficient [kg/$m^3{}_{octanol}$ per kg/ $m^3{}_{water}$]

K_{sw} : solid-water partitioning coefficient [kg/$kg_{solid\ phase}$ per kg/ $m^3{}_{water}$].

It needs to be stressed that the selection of a well predictive data estimation function for the solid-water partitioning coefficient is crucial as this is one of the most sensitive/important parameters in multimedia models when modelling semi-volatile organic substances (e.g., McKone, 1993b; Baker et al., 2001). As argued by Seth et al. (1999), class-specific regression models would be favourable. In particular, a separate relationship for Polycyclic Aromatic Hydrocarbons (PAHs) seems advisable (Chiou et al., 1998; Seth et al., 1999). A Quantitative Structure Activity Relationship (QSAR) that seems to be rather good in predicting K_{oc} values of (at least very hydrophobic) PAHs was presented by Baker et al. (2001). Although it is based on 'several easily calculable descriptors', the easiness comes with a profound knowledge of chemistry for deriving molecular connectivity indices which might not be available to all possible end users. Fairly recently, an entirely different approach has been proposed by Breivik and Wania (2003).

Trace elements

When acquiring data for heavy metals or trace elements, it is recommended to use solid-water partition coefficients (mostly referred to as K_d-values) of aged samples. 'Aged samples' means that the heavy metals applied to soil should be allowed some time to sorb to the soil matrix before the actual partitioning coefficient is determined.

Solid-water partition coefficients used

Within WATSON, the solid-water partition coefficients may be allowed to either depend on pH or on the organic carbon content, for trace elements or hydrophobic organic substances respectively. According to the prioritisation of substances (cf. section 3.2), the values used in this study are given in Table C-1.

Table C-1: pH-dependent solid-water partitioning coefficients (K_d) [$kg/kg_{solid\ phase}$ per $kg/m^3{}_{aqueous\ phase}$]

Trace element	pH range	K_d	Remarks
Arsenic	3.00 - 5.75	25.0	value for pH 4.9 adopted (United States - Environmental Protection Agency, 1998)
	5.75 - 6.25	26.9	geometric mean of value for pH 4.9 and 6.8 (United States - Environmental Protection Agency, 1998)
	6.25 - 7.25	29.0	value for pH 6.8 adopted (United States - Environmental Protection Agency, 1998)
	7.25 - 7.75	30.0	geometric mean of value for pH 6.8 and 8 (United States - Environmental Protection Agency, 1998)
	7.75 - 9.60	31.0	value for pH 8 adopted (United States - Environmental Protection Agency, 1998)
Cadmium	3.00 - 4.75	0.011	geometric mean of minimum and maximum value for pH 3-5 (Anonymous, 1999b)
	4.75 - 5.25	0.045	geometric mean of minimum and maximum values for pH 3-5 and 5-8 (Anonymous, 1999b)
	5.25 - 7.75	0.18	geometric mean of minimum and maximum value for pH 5-8 (Anonymous, 1999b)
	7.75 - 8.25	0.38	geometric mean of minimum and maximum values for pH 5-8 and 8-10 (Anonymous, 1999b)
	8.25 - 10.0	0.79	geometric mean of minimum and maximum value for pH 8-10 (Anonymous, 1999b)

Table C-1: pH-dependent solid-water partitioning coefficients (K_d) [$kg/kg_{solid\ phase}$ per $kg/m^3{}_{aqueous\ phase}$]

Trace element	pH range	K_d	Remarks
Chromium	3.00 - 5.75	1.20	value for pH 4.9 adopted, influence of competing anions and iron oxides not considered (United States - Environmental Protection Agency, 1998)
	5.75 - 6.25	46.5	geometric mean of value for pH 4.9 and 6.8, influence of competing anions and iron oxides not considered (United States - Environmental Protection Agency, 1998)
	6.25 - 7.25	1800	value for pH 6.8 adopted, influence of competing anions and iron oxides not considered (United States - Environmental Protection Agency, 1998)
	7.25 - 7.75	2782	geometric mean of value for pH 6.8 and 8, influence of competing anions and iron oxides not considered (United States - Environmental Protection Agency, 1998)
	7.75 - 9.60	4300	value for pH 8 adopted, influence of competing anions and iron oxides not considered (United States - Environmental Protection Agency, 1998)
Lead	3.75 - 6.75	0.88	geometric mean of minimum and maximum value for pH 4.0-6.3 and equilibrium lead concentrations of 1.0-99.9 μg/l (Anonymous, 1999b)
	6.75 - 8.75	3.11	geometric mean of minimum and maximum value for pH 6.4-8.7 and equilibrium lead concentrations of 1.0-99.9 μg/l (Anonymous, 1999b)
	8.75 - 11.0	7.01	geometric mean of minimum and maximum value for pH 8.7-11.0 and equilibrium lead concentrations of 1.0-99.9 μg/l (Anonymous, 1999b)

C.1.2 Air-water partitioning coefficient

The air-water partitioning coefficient is used when one has to deal with (semi-) volatile substances, i.e., those substances that have an appreciable vapour pressure at ambient temperatures. The (dimensionless) air-water partitioning coefficient can be derived from the Henry's law constant according to:

$$K_{aw,p} = \frac{H(p)}{R \cdot T(z)} \tag{C-3}$$

where

H	:	Henry's law constant of substance p [Pa $m^3{}_{water}$ per mol]
K_{aw}	:	air-water partitioning coefficient or dimensionless Henry's law constant of substance p [-]
R	:	universal gas constant [Pa $m^3{}_{gas}$ per K per mol]; 8.314510 (Lide, 2002)
T	:	absolute ambient temperature in zone z [K] (defined as described in section B.5.5).

The Henry's law constant of metals (except for mercury) and dissociated organic compounds are assumed to be negligible. These are set to zero.

C.1.3 Air-solid partitioning coefficient

Usually the partitioning between the aqueous phase on the one hand and the solid or gas phase on the other are known from which the air-solid partitioning coefficient can be derived. According to Gibbs' phase rule, the degree of freedom is the number of components (here: mole fractions) minus the number of phases (e.g., in aerated soils: three, in water bodies and sediments: two) plus a constant of two:

$$F = K - P + 2 \tag{C-4}$$

where:

F	:	Degrees of freedom
K	:	Number of components
P	:	Number of phases.

Assuming we have a system of three phases, i.e., the aqueous, the solid and the gas phase. A substance in the system may consequently have potentially three 'places' where it could stay. The three mole fractions are the components. If a substance partitions into each of these phases, the components equal the phases and the degree of freedom is always 2. This would be the case for a true multimedia substance, i.e., one that is volatile, soluble in water to some degree and that sorbs to solid phases. All three partitioning coefficients need to be known one of which is determined if the other two are known. If another substance avoids one of the phases the degree of freedom is always one as the number of components is smaller than the phases present in the system. The behaviour of such a substance is determined by the partitioning coefficient between the two phases in which it can be found. This is the case for example for non-volatile metals. If again another substance avoids two of the three phases then no partition coefficient needs to be known to determine the behaviour of the substance in the system.

Depending on the value of the air-water partitioning coefficient, the air-solid partitioning coefficient may also become zero for instance for metals (except for mercury) and dissociated organic substances.

C.2 Substance properties influencing the exposure

There are several substance-dependent parameters used in the exposure assessment. These may additionally depend on different exposure assessment frameworks. In the following, it is, therefore, distinguished whether the parameters for which the values will be given are used

- irrespective of the exposure assessment framework (section C.2.1),
- in relation to the Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities (HHRAP, United States - Environmental Protection Agency, 1998, section C.2.2), or
- by generic models for use in assessing the impact of discharges of radioactive substances to the environment (International Atomic Energy Agency, 2001, section C.2.3).

Note that the latter exposure assessment is less detailed than the former.

C.2.1 Exposure-related data independent of the exposure assessment framework used

In order to assess the effective Intake Fraction, it is necessary to define the mass fraction of a substance contained in food or ambient air that has the potential to exert an adverse effect. The values assumed are given in Table C-2.

Table C-2: Mass fraction of a substance contained in food leading to an effect ($fr\_w_{effective/total}$) [-]

Trace element	Exposure route	$fr\_w_{effective/total}$	Remarks
Arsenic	Ingestion	0.03	upper bound (Baxter and Lewis, 2002)
	Inhalation	1	inorganic forms of arsenic dominate the releases from high-temperature processes (Pacyna, 1987) which still appears to be valid today (Agency for Toxic Substances and Disease Registry, 2000b)
Cadmium	Ingestion	1	
	Inhalation	1	
Chromium	Ingestion	0.1	upper bound (Anonymous, 2002)
	Inhalation	0.1	only about 10-18 % of total chromium being emitted to air by oil and coal fired power plants as the primary source of particle-bound chromium to air is in the hexavalent state (French et al., 1998)
Lead	Ingestion	1	
	Inhalation	1	

C.2.2 Data related to the exposure assessment framework according to United States - Environmental Protection Agency (1998)

In the exposure assessment according to United States - Environmental Protection Agency (1998) several parameters are used which depend on the substance and sometimes also on the animal or plant through which humans are exposed (cf. section A.7). The values used are given in the following.

At equilibrium, the passive uptake of substances by an organism from its environment can be described with the help of the bioconcentration factor (BCF).

Table C-3: Bioconcentration factors (BCF) aqueous phase-freshwater fish [m^3/kg FW] (source: United States - Environmental Protection Agency, 1998)

Trace element	BCF	Remarks
Arsenic	0.02	Table A-3-14 (ibid.), BCF_{fish}, units adjusted
Cadmium	0.25	Table A-3-35 (ibid.), BCF_{fish}, units adjusted
Chromium	0.28	Table A-3-52 (ibid.), BCF_{fish}, units adjusted
Lead	0.008	Table A-3-128 (ibid.), BCF_{fish}, units adjusted, use of BAF instead of BCF

Depending on the medium from which the substances are taken up, one can distinguish BCFs for aquatic organisms from those for terrestrial organisms. Accordingly, the BCFs for fish and for vegetal produce are given separately in Tables C-3 and C-4, respectively.

Unlike passive uptake by plants and fish, farm animals actively take up feed and drinking water. In order to assess the concentration in animal products from daily pollutant intake at equilibrium, use is made of biotransfer factors (BTFs, Table C-5). Note the limited availability of BTFs for eggs, pork and poultry.

According to United States - Environmental Protection Agency (1998), uptake by root crops from soil is formulated in a K_{ow}-dependent way for any substance by introducing an empirical correction factor. Its value is 0.01 if the logarithm of the K_{ow} value is greater than 4 and 1 else. This is in line with the findings of Trapp (2002) for the dynamic case, however, at a different threshold. One may, therefore, consider to introduce a two-threshold approach where a correction factor of 0.1 could be used for instance at a log K_{ow} in the range of 2 to 4. Note that in the range between log K_{ow} from 1 or 2 to 4 the distribution behaviour of substances between aqueous phase and lipid phase of plants is in transition (cf. Figure 2 in Riederer, 1995).

As all trace elements considered in the present study have rather low values for K_{ow}, their correction factors are all set to unity (Table C-6).

Table C-4: Bioconcentration factors (BCF) for different vegetal produce [mol/kg plant DW per mol/kg soil DW] (source: United States - Environmental Protection Agency, 1998)

Trace element	Produce	BCF	Remarks
Arsenic	Aboveground exposed produce	0.013	Table A-3-14, Br_{ag}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.)
	Belowground produce	0.016	Table A-3-14, $Br_{rootveg}$, adapted to 30 cm soil depth (see comment on page A-3-19, ibid.)
	Cereals	0.008	Table A-3-14, Br_{grain}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.)
	Grass, forage	0.072	Table A-3-14, Br_{forage}, adapted to 30 cm soil depth (see comment on page A-3-2, ibid.1)
	Silage	0.072	Table A-3-14, Br_{forage}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.), value also applies to silage
Cadmium	Aboveground exposed produce	0.25	Table A-3-35, Br_{ag}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.)
	Belowground produce	0.13	Table A-3-35, $Br_{rootveg}$, adapted to 30 cm soil depth (see comment on page A-3-19, ibid.)
	Cereals	0.12	Table A-3-35, Br_{grain}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.)
	Grass, forage	0.73	Table A-3-35, Br_{forage}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.)
	Silage	0.73	Table A-3-35, Br_{forage}, adapted to 30 cm soil depth (see comment on page A-3-21, ibid.), value also applies to silage

Table C-4: Bioconcentration factors (BCF) for different vegetal produce [mol/kg plant DW per mol/kg soil DW] (source: United States - Environmental Protection Agency, 1998)

Trace element	Produce	BCF	Remarks
Chromium	Aboveground exposed produce	0.0049	Table A-3-52, Br_{ag}
	Belowground produce	0.0045	Table A-3-52, $Br_{rootveg}$
	Cereals	0.0045	Table A-3-52, Br_{grain}
	Grass, forage	0.0075	Table A-3-52, Br_{forage}
	Silage	0.0075	Table A-3-52, Br_{forage}, value also applies to silage
Lead	Aboveground exposed produce	0.014	Table A-3-128, Br_{ag}
	Belowground produce	0.009	Table A-3-128, $Br_{rootveg}$
	Cereals	0.009	Table A-3-128, Br_{grain}
	Grass, forage	0.045	Table A-3-128, Br_{forage}
	Silage	0.045	Table A-3-128, Br_{forage}, value also applies to silage

Table C-5: Biotransfer factors (BTF) relating daily pollutant intake to contents in animal produce [s·capita/kg FW] (source: United States - Environmental Protection Agency, 1998)

Trace element	Produce	BTF	Remarks
Arsenic	Beef and veal	173	Table A-3-14, Ba_{beef}, units adjusted
	Cow milk and products	518	Table A-3-14, Ba_{milk}, units adjusted
	Eggs	n/a	Table A-3-14, Ba_{egg}, not defined
	Pork	n/a	Table A-3-14, Ba_{pork}, not defined
	Poultry	n/a	Table A-3-14, $Ba_{chicken}$, not defined
Cadmium	Beef and veal	10.4	Table A-3-35, Ba_{beef}, units adjusted
	Cow milk and products	0.56	Table A-3-35, Ba_{milk}, units adjusted
	Eggs	216	Table A-3-35, Ba_{egg}, units adjusted
	Pork	16.5	Table A-3-35, Ba_{pork}, units adjusted
	Poultry	9158	Table A-3-35, $Ba_{chicken}$, units adjusted
Chromium	Beef and veal	475	Table A-3-52, Ba_{beef}, units adjusted
	Cow milk and products	130	Table A-3-52, Ba_{milk}, units adjusted
	Eggs	n/a	Table A-3-52, Ba_{egg}, not defined
	Pork	n/a	Table A-3-52, Ba_{pork}, not defined
	Poultry	n/a	Table A-3-52, $Ba_{chicken}$, not defined
Lead	Beef and veal	25.9	Table A-3-128, Ba_{beef}, units adjusted
	Cow milk and products	21.6	Table A-3-128, Ba_{milk}, units adjusted

Table C-5: Biotransfer factors (BTF) relating daily pollutant intake to contents in animal produce [s·capita/kg FW] (source: United States - Environmental Protection Agency, 1998)

Trace element	Produce	BTF	Remarks
Lead (continued)	Eggs	n/a	Table A-3-128, Ba_{egg}, not defined
	Pork	n/a	Table A-3-128, Ba_{pork}, not defined
	Poultry	n/a	Table A-3-128, $Ba_{chicken}$, not defined

Table C-6: Empirical correction factor ($emp_{BCF, root\ crop}$) for equilibrium uptake by belowground produce depending on the substance's octanol-water partitioning coefficient (K_{ow}) [-] (source: United States - Environmental Protection Agency, 1998, p. 5-35)

Trace element	$emp_{BCF, root\ crop}$
Arsenic	1
Cadmium	1
Chromium	1
Lead	1

Table C-7: Mass fraction adhering to aboveground exposed produce during wet deposition ($fr\_w_{adhere/wet\ deposition}$) [-] (source: United States - Environmental Protection Agency, 1998, Table B-2-7, p. B-78; value for cations and insoluble particles)

Trace element	$fr\_w_{adhere/wet\ deposition}$
Arsenic	0.6
Cadmium	0.6
Chromium	0.6
Lead	0.6

The exposure assessment by United States - Environmental Protection Agency (1998), furthermore, distinguishes between cations and anions in terms of their adhesion to vegetal surfaces upon intercepted wet deposition (Table C-7).

C.2.3 Data related to the exposure assessment framework according to International Atomic Energy Agency (2001)

During model evaluation, a second exposure assessment framework has been employed (cf. Table 9-4). Table C-8 provides the corresponding values used.

Table C-8: Parameter values used for the exposure assessment according to International Atomic Energy Agency (2001)

Trace element	Parameter	Unit	Receptors	Value[a]
Cadmium	bioconcentration factor for aboveground produce	mol/kg plant DW per mol/kg soil DW	Grass, forage	5
	bioconcentration factor soil-plant	mol/kg plant FW per mol/kg soil DW	All crops considered	0.5
	biotransfer factor daily pollutant intake to milk	s/m^3	Cow milk and products	1728000
	biotransfer factor relating daily pollutant intake to meat	s·capita/kg FW	Beef and veal	86.4
Lead	bioconcentration factor for aboveground produce	mol/kg plant DW per mol/kg soil DW	Grass, forage	0.1
	bioconcentration factor soil-plant	mol/kg plant FW per mol/kg soil DW	All crops considered	0.02
	biotransfer factor daily pollutant intake to milk	s/m^3	Cow milk and products	25920
	biotransfer factor relating daily pollutant intake to meat	s·capita/kg FW	Beef and veal	60.48

a.Found in Table XI, adherent soil particles are included.

C.3 Monitoring data on media and food concentrations

In Chapter 9, a comparison of the model results in terms of concentrations in different media and foodstuff with measured data has been carried out. The monitoring data as used in the Figures 9-3 through 9-6 are taken from the data compiled in Tables C-9 through C-12 for arsenic, cadmium, chromium and lead, respectively. The values used are highlighted in bold. If the lower limit was reported to be below the detection limit (indicated by a '<' before the numbers), half of that value was taken.

Table C-9: Reported arsenic concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Upper continental crust	expectation value/range	**2.0**	[mg/kg]	Table 1 (Wedepohl, 1995); natural background value
Any soil	total range	**0.07-95**	[mg/kg DW]	Table 120 (Kabata-Pendias and Pendias, 2001); minimum and maximum values in Fig. 9-3
		<0.2-83	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998)
	expectation value/range	0.1-20	[mg/kg]	Gebel (1999)
		0.5-**6.6**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-3
		0.2-41	[mg/kg DW]	arithmetic mean, Table 120 (Kabata-Pendias and Pendias, 2001)
	maximum value due to local contamination	100-2500	[mg/kg]	copper processing (Gebel, 1999)
		2500	[mg/kg DW]	metal processing, Table 121 (Kabata-Pendias and Pendias, 2001)
		2000	[mg/kg DW]	chemical works, Table 121 (Kabata-Pendias and Pendias, 2001)
Agricultural soil	total range	**<0.2-19**	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-3

Table C-9: Reported arsenic concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Agricultural soil (continued)	expectation value/range	**1.55-6.6**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-3 obtained by averaging
	maximum value due to local contamination	700	[mg/kg]	arsenic-containing herbicide application (Gebel, 1999)
		625	[mg/kg DW]	application of arsenical pesticides, Table 121 (Kabata-Pendias and Pendias, 2001)
Surface water	total range	$\mathbf{<1 \cdot 10^{-5} - 2.5 \cdot 10^{-2}}$	[mg/l]	unfiltered samples (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-3
	expectation value/range	$\mathbf{2 \cdot 10^{-4} - 1.4 \cdot 10^{-3}}$	[mg/l]	median range, unfiltered samples (Reimann and de Caritat, 1998); median value in Fig. 9-3 obtained by averaging
Sediments	total range	**<2-1305**	[mg/kg DW]	only particles smaller than 0.18 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-3
	expectation value/range	**2-12**	[mg/kg DW]	median range, only particles smaller than 0.18 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-3 obtained by averaging
Cereals	total range	**<0.1-365**	[µg/kg FW]	range for baking goods and cereals, Table 1 (Gebel, 1999); minimum and maximum values in Fig. 9-3

Table C-9: Reported arsenic concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Cereals (continued)	expectation value/range	**24.5**	[µg/kg FW]	arithmetic mean for baking goods and cereals, Table 1 (Gebel, 1999); 'median' value in Fig. 9-3
		0.3-40	[µg/kg FW]	Table 122 (Kabata-Pendias and Pendias, 2001) [a]
Potatoes	expectation value/range	**14.2**	[µg/kg FW]	arithmetic mean, baked potatoes, Table 1 (Gebel, 1999); 'median' value in Fig. 9-3
		5.0-33.4	[µg/kg FW]	Table 122 (Kabata-Pendias and Pendias, 2001); minimum and maximum values in Fig. 9-3 [a]
	maximum value	183	[µg/kg FW]	tuber peels after application of arsenical pesticides, Table 123 (Kabata-Pendias and Pendias, 2001) [a]
Vegetables	total range	<0.1-84	[µg/kg FW]	range, Table 1 (Gebel, 1999)
	expectation value/range	7.0	[µg/kg FW]	arithmetic mean, Table 1 (Gebel, 1999)
Spinach	expectation value/range	**16.8-126**	[µg/kg FW]	Table 122 (Kabata-Pendias and Pendias, 2001) [a]; minimum and maximum values in Fig. 9-3; 'median' value in Fig. 9-3 obtained by averaging

Table C-9: Reported arsenic concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Freshwater fish	total range	**29-555**	[µg/kg FW]	range, Table 1 (Gebel, 1999); minimum and maximum values in Fig. 9-3
	expectation value/range	**160**	[µg/kg FW]	arithmetic mean, Table 1 (Gebel, 1999); 'median' value in Fig. 9-3
Milk and dairy products	total range	**<0.4-26.0**	[µg/kg FW]	range, Table 1 (Gebel, 1999); minimum and maximum values in Fig. 9-3
	expectation value/range	**33.8**	[µg/kg FW]	arithmetic mean, Table 1 (Gebel, 1999); 'median' value in Fig. 9-3
Meat	expectation value/range	**6**	[µg/kg FW]	arithmetic mean, Table 1 (Gebel, 1999); 'median' value in Fig. 9-3
Poultry	expectation value/range	35.9	[µg/kg FW]	arithmetic mean, Table 1 (Gebel, 1999)

a. Converted from mg/kg DW into mg/kg FW according to mass fractions of food dry matter (cf. Table B-22).

Table C-10: Reported cadmium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Upper continental crust	expectation value/range	**0.102**	[mg/kg]	Table 1 (Wedepohl, 1995); natural background value
Any soil	total range	**<0.01-40.9**	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-4
		0.01-4	[mg/kg DW]	Table 71 (Kabata-Pendias and Pendias, 2001)
	expectation value/range	0.117-**0.7**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-4
		0.06-1.1	[mg/kg DW]	arithmetic mean, Table 71 (Kabata-Pendias and Pendias, 2001)
		<0.01-0.5	[mg/kg DW]	Table 8.1 (Stoeppler, 1992)
	maximum value due to local contamination	1781	[mg/kg DW]	metal processing, Table 72 (Kabata-Pendias and Pendias, 2001)
		10	[mg/kg DW]	roadside, Table 72 (Kabata-Pendias and Pendias, 2001)
		<0.2- >50	[mg/kg DW]	typical polluted value, Table 8.1 (Stoeppler, 1992)
Agricultural soil	total range	**<0.01-3.8**	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-4
		0.037-0.908	[mg/kg DW]	Table 2.8 (Traina, 1999)

Table C-10: Reported cadmium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Agricultural soil (continued)	expectation value/range	0.117-**0.3**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-4
		0.2-1.0	[mg/kg]	rural areas, Table 1 (Ewers and Wilhelm, 1995)
		0.5-1.5	[mg/kg]	urban areas, Table 1 (Ewers and Wilhelm, 1995)
	maximum value due to local contamination	167	[mg/kg DW]	sludged, irrigated, or fertilized farmland, Table 72 (Kabata-Pendias and Pendias, 2001)
Surface water	total range	$\mathbf{<2 \cdot 10^{-6}-9.6 \cdot 10^{-3}}$	[mg/l]	unfiltered samples (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-4
	expectation value/range	$\mathbf{<2 \cdot 10^{-5}-2.9 \cdot 10^{-4}}$	[mg/l]	median range, unfiltered samples (Reimann and de Caritat, 1998); median value in Fig. 9-4 obtained by averaging
		$<5 \cdot 10^{-5}-2 \cdot 10^{-4}$	[mg/l]	dissolved and particulate bound, Table 8.1 (Stoeppler, 1992)
		$1 \cdot 10^{-5}-4 \cdot 10^{-5}$	[mg/l]	Table 1 (Ewers and Wilhelm, 1995)
River sediments	expectation value/range	**0.04-0.8**	[mg/kg DW]	Table 8.1 (Stoeppler, 1992); minimum and maximum values in Fig. 9-4; median value in Fig. 9-4 obtained by averaging

Table C-10: Reported cadmium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
River sediments (continued)	maximum value due to local contamination	30-800	[mg/kg DW]	typical polluted value, Table 8.1 (Stoeppler, 1992)
Cereals	total range	**<0.0011-1.44**	[mg/kg FW]	Table 75 (Kabata-Pendias and Pendias, 2001); minimum and maximum values in Fig. 9-4 [a]
	expectation value/range	**0.012-0.244**	[mg/kg FW]	median range, Table 75 (Kabata-Pendias and Pendias, 2001); median value in Fig. 9-4 obtained by averaging [a]
		≤0.04	[mg/kg FW]	wheat flour, wheat bread, bran, potatoes root and foliage vegetables, rice, Table 8.1 (Stoeppler, 1992)
Potatoes	total range	**0.0003-0.435**	[mg/kg FW]	Table 2 (Ewers and Wilhelm, 1995); minimum and maximum values in Fig. 9-4
	expectation value/range	**0.001-0.09**	[mg/kg FW]	median range, Table 73 (Kabata-Pendias and Pendias, 2001); median value in Fig. 9-4 obtained by averaging
		≤0.04	[mg/kg FW]	wheat flour, wheat bread, bran, potatoes root and foliage vegetables, rice, Table 8.1 (Stoeppler, 1992)
		0.016	[mg/kg FW]	median, Table 2 (Ewers and Wilhelm, 1995)

Table C-10: Reported cadmium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Spinach leaves	maximum value due to local contamination	**0.33** - 0.54	[mg/kg FW]	Table 74 (Kabata-Pendias and Pendias, 2001); 'median' value in Fig. 9-4 [a]
Fish	expectation value/range	**<0.0025**	[mg/kg FW]	fish muscle, Table 8.1 (Stoeppler, 1992); median value in Fig. 9-4 [a]
Meat	expectation value/range	**≤0.005**	[mg/kg FW]	meat from various animals, Table 8.1 (Stoeppler, 1992); median value in Fig. 9-4
		<0.05	[mg/kg FW]	Ewers and Wilhelm (1995)
Eggs	expectation value/range	**<0.05**	[mg/kg FW]	Ewers and Wilhelm (1995); median value in Fig. 9-4
Milk and dairy products	expectation value/range	**≤0.001**	[mg/kg FW]	Table 8.1 (Stoeppler, 1992); median value in Fig. 9-4
		<0.05	[mg/kg FW]	Ewers and Wilhelm (1995)

a. Converted from mg/kg DW into mg/kg FW according to mass fractions of food dry matter (cf. Table B-22).

Table C-11: Reported chromium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Upper continental crust	expectation value/range	**35**	[mg/kg]	Table 1 (Wedepohl, 1995); natural background value
Any soil	total range	1-**1500**	[mg/kg DW]	Table 137 (Kabata-Pendias and Pendias, 2001); maximum value in Fig. 9-5
		0.2-838	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); minimum value in Fig. 9-5
	expectation value/range	19.1-**80**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-5
		10-90	[mg/kg]	Table 1 on environmental loads (Hertl and Merk, 1999); values may, therefore, represent expectation values of non-pristine soils
		7-221	[mg/kg DW]	arithmetic mean, Table 137 (Kabata-Pendias and Pendias, 2001)
Agricultural soil	total range	**<5-510**	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-5
	expectation value/range	**19.1-57**	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998); median value in Fig. 9-5 obtained by averaging
Surface water	total range	**$<1 \cdot 10^{-4}$ - 0.179**	[mg/l]	unfiltered samples (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-5

Table C-11: Reported chromium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Surface water (contin-ued)	expectation value/range	0.001-0.01	[mg/l]	Table 1 on environmental loads (Hertl and Merk, 1999); values may, therefore, represent expectation values of non-pristine freshwater
		$<1 \cdot 10^{-4}$ - $9.7 \cdot 10^{-3}$	[mg/l]	median range, unfiltered samples (Reimann and de Caritat, 1998); median value in Fig. 9-5 obtained by averaging
Sediments	total range	**<5-3176**	[mg/kg DW]	only particles smaller than 0.18 mm considered (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-5
	expectation value/range	**64-161**	[mg/kg DW]	median range, only particles smaller than 0.18 mm considered (Reimann and de Caritat, 1998); 'median' value in Fig. 9-5 obtained by averaging
Cereals	expectation value/range	4	[µg/kg]	Hertl and Merk (1999) [a,b]
		1.4-55	[µg/kg FW]	Table 138 (Kabata-Pendias and Pendias, 2001) [b]; minimum and maximum values in Fig. 9-5; 'median' value in Fig. 9-5 obtained by averaging
Potatoes	expectation value/range	**3.5**	[µg/kg FW]	Table 138 (Kabata-Pendias and Pendias, 2001) [b]; median value in Fig. 9-5
Vegetables	expectation value/range	**2.5**	[µg/kg]	Hertl and Merk (1999) [a,b]; median value in Fig. 9-5

Table C-11: Reported chromium concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Freshwater fish	expectation value/range	**27.2**	[µg/kg]	Hertl and Merk (1999) [a,b]; median value in Fig. 9-5
Milk and dairy products	expectation value/range	**100**	[µg/kg]	Hertl and Merk (1999) [a]; median value in Fig. 9-5
Meat	expectation value/range	**78.8**	[µg/kg]	Hertl and Merk (1999) [a,b]; median value in Fig. 9-5

a. There is neither an indication of whether the concentration is given for fresh or dry weight nor whether the values are representative for 'pristine' or contaminated situations; it is assumed that the concentrations provided for foodstuff other than milk and dairy products is on a dry weight-basis.

b. Converted from mg/kg DW into mg/kg FW according to mass fractions of food dry matter (cf. Table B-22).

Table C-12: Reported lead concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Upper continental crust	expectation value/range	**17**	[mg/kg]	Table 1 (Wedepohl, 1995); natural background value
Any soil	total range	3-16338	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998)
		1.5-286	[mg/kg DW]	Table 110 (Kabata-Pendias and Pendias, 2001)
		1.5-888	[mg/kg DW]	Table 2.21 (Nriagu, 1978); minimum and maximum values in Fig. 9-6
	expectation value/range	7.45-40	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998)
		7.9-84	[mg/kg DW]	arithmetic mean, Table 110 (Kabata-Pendias and Pendias, 2001); 'median' value in Fig. 9-6 obtained by averaging
	maximum value due to local contamination	18500	[mg/kg DW]	metal processing, Table 111 (Kabata-Pendias and Pendias, 2001)
		30000	[mg/kg DW]	'geologically polluted' soils, Table 2.11 (Nriagu, 1978)
		7000	[mg/kg DW]	roadside, Table 111 (Kabata-Pendias and Pendias, 2001)
Agricultural soil	total range	3-192	[mg/kg DW]	only top soils and particles smaller than 2 mm considered (Reimann and de Caritat, 1998)

Table C-12: Reported lead concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Agricul-tural soil (contin-ued)	total range (continued)	**1.5-888**	[mg/kg DW]	Table 2.21 (Nriagu, 1978); minimum and maximum values in Fig. 9-6
	expectation value/range	7.45-14	[mg/kg DW]	median range; only top soils and particles smaller than 2 mm consid-ered (Reimann and de Caritat, 1998)
		10-247	[mg/kg DW]	Table 2.21 (Nriagu, 1978); 'median' value in Fig. 9-6 obtained by averaging
	maximum value due to local contam-ination	3916	[mg/kg DW]	sludged farmland, Table 111 (Kabata-Pendias and Pendias, 2001)
Surface water	total range	**$<10^{-5}$-0.58**	[mg/l]	unfiltered samples (Reimann and de Caritat, 1998); minimum and maximum values in Fig. 9-6
	expectation value/range	**$2.1 \cdot 10^{-4}$-$3.4 \cdot 10^{-3}$**	[mg/l]	median range, unfiltered samples (Reimann and de Caritat, 1998); 'median' value in Fig. 9-6 obtained by averaging
Lake sedi-ments	total range	**<0.1-5000**	[mg/kg DW]	Nriagu (1978); minimum and maximum values in Fig. 9-6

Table C-12: Reported lead concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Lake sediments (continued)	expectation value/range	**16**	[mg/kg DW]	Nriagu (1978); 'median' value in Fig. 9-6 obtained by averaging the lake value with the river value
		95	[mg/kg DW]	average lake sediment concentration with evidence of pollution (Nriagu, 1978)
River sediments	total range	3.9-3700	[mg/kg DW]	Table 2.29 (Nriagu, 1978)
	expectation value/range	**23**	[mg/kg DW]	Nriagu (1978); 'median' value in Fig. 9-6 obtained by averaging the lake value with the river value
		98	[mg/kg DW]	average riverine sediment concentration with evidence of pollution (Nriagu, 1978)
Cereals	total range	**<0.01-40**	[mg/kg FW]	Table 113 (Kabata-Pendias and Pendias, 2001) [a]; minimum and maximum values in Fig. 9-6
	expectation value/range	0.01-0.71	[mg/kg FW]	arithmetic mean range, Table 113 (Kabata-Pendias and Pendias, 2001) [a]
		0.05-**0.06**	[mg/kg FW]	median, Table 2b (Wilhelm and Ewers, 1999); median value in Fig. 9-6
	maximum value	0.45	[mg/kg FW]	98^{th} percentile, Table 2b (Wilhelm and Ewers, 1999)
		40	[mg/kg FW]	Table 113 (Kabata-Pendias and Pendias, 2001) [a]

Table C-12: Reported lead concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Potatoes	expectation value/range	**0.08-0.50**	[mg/kg FW]	arithmetic mean range, Table 112 (Kabata-Pendias and Pendias, 2001) [a]; maximum and 'median' values in Fig. 9-6
		0.03	[mg/kg FW]	median, Table 2b (Wilhelm and Ewers, 1999); minimum value in Fig. 9-6
	maximum value	0.19	[mg/kg FW]	98^{th} percentile, Table 2b (Wilhelm and Ewers, 1999)
		425	[mg/kg AW]	metal processing, ash weight basis, Table 115 (Kabata-Pendias and Pendias, 2001)
Leafy vegetables	expectation value/range	**0.04**	[mg/kg FW]	median, Table 2b (Wilhelm and Ewers, 1999); median value in Fig. 9-6
	maximum value	0.81	[mg/kg FW]	98^{th} percentile, Table 2b (Wilhelm and Ewers, 1999)
		27.1	[mg/kg FW]	metal processing, Table 115 (Kabata-Pendias and Pendias, 2001) [a]
Fish	expectation value/range	**0.03**	[mg/kg FW]	median, Table 2a (Wilhelm and Ewers, 1999); median value in Fig. 9-6
	maximum value	0.37	[mg/kg FW]	98^{th} percentile, Table 2a (Wilhelm and Ewers, 1999)
Eggs	expectation value/range	0.02	[mg/kg FW]	median, Table 2a (Wilhelm and Ewers, 1999)

Table C-12: Reported lead concentrations in environmental media and foodstuff

Medium or food item	Type of value	Value	Unit	Remarks
Eggs (continued)	maximum value	0.46	[mg/kg FW]	98th percentile, Table 2a (Wilhelm and Ewers, 1999)
Milk and dairy products	expectation value/range	0.01	[mg/l]	median for milk, Table 2a (Wilhelm and Ewers, 1999)
		0.07	[mg/kg FW]	median for cheese, Table 2a (Wilhelm and Ewers, 1999); median value in Fig. 9-6
	maximum value	0.04	[mg/l]	98th percentile for milk, Table 2a (Wilhelm and Ewers, 1999)
		1.17	[mg/kg FW]	98th percentile for cheese, Table 2a (Wilhelm and Ewers, 1999)
Pork	expectation value/range	**0.08**	[mg/kg FW]	median, Table 2a (Wilhelm and Ewers, 1999); median value for beef in Fig. 9-6
	maximum value	0.53	[mg/kg FW]	98th percentile, Table 2a (Wilhelm and Ewers, 1999)

a. Converted from mg/kg DW into mg/kg FW according to mass fractions of food dry matter (cf. Table B-22).