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Ranking of chemical substances based on the Japanese Pollutant Release and Transfer Register using partial order theory and random linear extensions

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Abstract

In 1997 a Pollutant Release and Transfer Register (PRTR) pilot project was initiated in Japan. In 1998 the project was expanded and in 1999 a law concerning the establishment of a national PRTR was adopted. Data on the emissions of chemical substances are therefore now being reported on a continuous base. In relation to the PRTR project data on toxicity have been collected. In order to make efficient use of the collected information on emission and toxicity it is useful to group or rank the chemical substances according to the impact on human health and the environment.

It has recently been argued that partial order theory (POT) in combination with the use of linear extensions (LE) may be the most objective way to create a linear rank. The methodology has been further expanded to handle larger data sets by the use of random linear extensions (RLE). In this paper the Japanese PRTR data are ranked using the POT/RLE methodology.

An average rank is established for chemical substances in the 1998 and 1999 PRTR in Japan. The top 10 chemical substances in the 1998 PRTR are: dichlorvos, inorganic arsenic compounds, cobalt compounds, beryllium compounds, fenitrothion, disulfoton, parathion, diazinon, 4,4′-diamino-3,3′-dichlorodiphenylmethane and antimony compounds. The top 10 chemical substances from the 1999 PRTR are PCBs, lead compounds, fenitrothion, dichlorvos, disulfoton, inorganic arsenic compounds, chlorothalonil, thiobencarb, chromium and HCFC-141b.

The descriptor having the highest influence on the ranking of the 1998 PRTR data is the production volume, which, however, is not given in the 1999 PRTR. Further, the disagreement between the ranking with the lack of toxicity data substituted with mean and maximum values, respectively, strongly indicates a general need for further toxicological investigations.

Keywords: PRTR, Pollutant Release and Transfer Register; Emissions; Random linear extensions; Hasse diagram; Partial order theory; Ranking; Chemical substances

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1. Introduction

In Japan the emissions of chemical substances are controlled either indirectly (e.g. through regulation on concentrations in water or air), specifically (such as regulation for PCBs, mercury compounds, dioxins, agricultural chemicals or CFCs) or in other types of regulation (e.g. concerning material safety data sheets or prevention of major industrial accidents). Despite the current regulation, enhanced production and use of chemical substances has caused an increase in the emissions, which present risks to human health and the environment (Environmental Agency of Japan, 1997). The Environmental Agency of Japan stated that there was not adequate knowledge on these emissions and the associated risks in Japan. Besides the annual surveys on chemical substances in the environment the most prominent effort to gain knowledge on the emissions of chemical substances in Japan is the establishment of the Japanese Pollutant Release and Transfer Register (PRTR). A PRTR is an inventory of releases to air, water and soil of potentially harmful chemical substances as well as chemical substances transported off site for treatment or disposal (OECD, 2000). A PRTR system allows environmental policymakers to track the generation and release of pollutants over time. It can thus be an important tool for the regulators in the formulation of overall political objectives since it provide a baseline of data and information.

In 1997 a PRTR pilot project was initiated in Japan. In 1998 the project was further expanded and in 1999 a new law concerning the establishment of a national PRTR was passed. Data on the emissions of chemical substances are therefore now being reported regularly. In relation to the PRTR project data on toxicity has been collected (Urano, 2001).

However in order to make efficient use of the collected information on emission and toxicity it is useful to group or rank the chemical substances according to the impact on human health and the environment.

It has recently been argued that partial order theory (POT) in combination with the use of linear extensions (LE) may be the most objective way to rank a set of elements. This was concluded by Lerche et al. (2002b) who compared the POT/LE methodology with other types of multi-criteria analysis (MCA), such as e.g. aggregation of the descriptors. The objectivity lies in the fact that in contrast to other MCA methodologies, there is no need to unify the descriptors using weighting coefficients in any kind of functional relationships. Further, the result can be given as ranking probabilities, giving a more detailed picture than the simple statement of the rank provided by most MCAs. Despite the attractiveness of the POT/LE approach, it has, due to combinatorial problems, been virtually impossible to apply the methodology on data sets including more than approximately 12–15 chemical substances. However, recently an iterative methodology based on Random Linear Extensions (RLE) has been developed (Sørensen et al., 2001; Lerche and Sørensen, 2003). This expands the application of the methodology to data set including up to approximately 1000 chemical substances. The method was further improved by a better estimations of the starting configuration of the iterative procedure (Lerche et al., 2003). This paper on the Japanese PRTR data presents the first application of the improved methodology.

The objective of the present study is to apply the POT/RLE approach to rank the chemical substances from the Japanese PRTR applying the POT/RLE methodology. The intention is on one hand to illustrate the capability of the POT/RLE method and on the other hand to provide the Japanese Environmental Agency with results to be used in the policy making process. The study further evaluates the influence from the various descriptors and the lack of data on toxicity. Finally, the result of this study is seen in relation to quantitative estimations of the environmental concentrations for 68 chemical substances from the Japanese PRTR database (Kawamoto et al., 2001).

2. The Japanese Pollutant Release and Transfer Register

A Pollutant Release and Transfer Register (PRTR) is an innovative method of promoting environmental risk management of chemical substances involving the stakeholders more directly. Facilities releasing chemical substances listed in the PRTR are to report periodically what pollutants are released, the quantity and to which environmental media. Data is then made available to interested parties including the public. In addition PRTR can be designed to include estimates from non-point sources, such as agriculture and transportation.

In 1992 the PRTR concept was an outcome of the United Nations Conference on Environment and Development (UNCED) in Rio de Janeiro. The conference mission statement, Agenda 21, lists a set of specific objectives. One of these objective was for governments to implement and improve databases and inventories on chemical emissions. Further, this information should be available to the general public.

Following, the PRTR concept was introduced within the Chemicals Programme under the Environmental Health and Safety unit of the Organisation for Economic Co-operation and Development (OECD, 2000). In 1996 after the development of suitable guidelines, the OECD Council issued a recommendation to initiate the establishment of PRTRs in the member states. Several countries, including the United States (as the Toxic Release Inventory), Canada, The Netherlands and United Kingdom (as the Chemical Release Inventory) have already introduced PRTRs.

Lately, under the 1998 Convention on Access to Information, Public Participation in Decision Making and Access to Justice in Environmental Matters, also known as the Aarhus Convention, under the United Nation Economic Commission for Europe (UN-ECE) a draft PRTR protocol has been adopted at the Kiev Ministerial Conference in May 2003.

Following the international recommendations the Environmental Agency of Japan initiated a pilot PRTR project in 1997 (The Japanese Ministry of Environment, 2001a). The project involved 1700 businesses in Kanagawa and Aichi prefectures and targeted 178 chemical substances. In addition to the reporting of the annual volumes released from the companies, the production volume and figures on usage, the government estimated the release from non-point sources (Masuzawa, 1997). The choice of the 178 chemical substances included in the pilot project was based on PRTRs in other countries and on toxicity data and production volume.

In 1998 the Japanese Environmental Agency hosted the OECD International Conference on PRTR (www.oecd.org/eks/prtr). Further, the PRTR project was expanded to include 354 chemical substances and cover most of Japan. Finally, in 1999 the Japanese Government established a new law concerning a national PRTR. As the PRTR data are being collected they are made available to the public. However in this study only data from 1998 and 1999 (the first two years of reporting) are applied. Since PRTR data are being published continuously as they are collected more recent data may be available. However, applying the presented methodology these data can easily be ranked as they are coming forth. Here the main focus is not to rank the very latest data, but to provide the policymakers with a tool that can be used continuously.

Considering the 1998 data, of the original 178 chemical substances in the PRTR only emissions on 137 were reported. For the 354 chemical substances in the 1999 PRTR only emissions on 302 chemical substances were reported (The Japanese Ministry of Environment, 2001a,b).

In order to give the reader the possibility to follow the calculations in detail the 1998 data are given in the appendix. The data for 1999 can be found in the reference (The Japanese Ministry of Environment, 2001a,b). In Appendix A the emissions reported by facilities are separated into seven categories (emission to air, water or soil, transfer to sewage, waste (incineration) or landfill and recycling). In Appendix B production and usage volume are reported together with estimation of emission from five non-point sources (emission due to use as pesticide, due to transportation, from households and offices, from non-regulated industry and disperse waste). Both in Appendices A and B when a 0 is given in the table it indicates that no emission has been reported or estimated. The release categories are presented in Table 1 together with the "top scores" i.e. the chemicals with the highest emissions.

The release categories for the 1999 emission data are different from the 1998 data. The 1999 categories are presented in Table 2. Notice that production, use and recycling is not included in the 1999 survey. Instead emission to sewage has been separated into emission from public and private sewage treatment plants.

In relation to the PRTR project in Japan data on toxicity for 435 substances were collected (Urano, 2001). The toxicity data were extracted from official report or authorised documents from the Japanese Government, the World Health Organisation, International Agency for Research on Cancers, EU or the USA Environmental Protection Agency. Urano (2001) gave the substances scores from +A to E (+A,A,B,C,D,E) for seven types of toxicity (chronic oral toxicity, chronic inhalation toxicity, carcinogenecity, reproductive disorder, mutagenecity, allergic response and aquatic ecotoxicity). In this study the letter classification (+A,A,B,C,D,E) has

Table 1
Emission categories and top scores for the 1998 PRTR

	Release category	Max (ton)	Top score
1	Production volume	795 000.0	Xylene (mixed isomers)
2	Use	466 000.0	Xylene (mixed isomers)
3	Emission to air	7330.0	Toluene
4	Emission to water	219.0	Nitrobenzene
5	Emission to soil	0.2	Toluene
6	Transfer to sewage	19.0	Ethanal amine
7	Transfer to waste	1220.0	Toluene
8	Transfer to landfill	249.0	Nickel compounds
9	Recycling	4570.0	Chromium compounds (excl. hexavalent)
10	Emission as pesticide	135.0	1,3-Dichloropropene
11	Emission transportation	227.0	Formaldehyde
12	Emission household/offices	836.0	Xylene (mixed isomers)
13	Emission non-regulated industry	113.0	Xylene (mixed isomers)
14	Dispersive waste	267.0	Zinc compounds

Table 2
Emission categories and top scores for the 1999 PRTR

	Release category	Max (ton)	Top score
1	Emission to air	22 350.0	Toluene
2	Emission to water	28 750.0	PCB
3	Emission to soil	7.5	Chromium
4	Transfer to landfill	4795.0	Arsenic
5	Transfer to solid waste	14 056.7	Manganese
6	Transfer to public STP	486.3	*N*,*N*-dimethylformamide
7	Transfer to company STP	130.0	Toluene
8	Emission as pesticide	940.0	*D*,*D*-1,3-dichloropropene
9	Emission transportation	1530.0	Formaldehyde
10	Emission household/offices	3600.0	Xylene
11	Emission non-regulated industry	2510.0	Xylene

been replaced by values descending from 6 to 1, i.e. +A is equal to 6 being the most toxic classs, A is equal to 5 etc. There are six types of human toxicity and one type of ecotoxicity inevitable putting a focus on the protection human health.

The scores were not only given according to the strength of toxicity since e.g. a substance is normally either carcinogenic or not, but also according to the validity of the result. See Urano (2001) for a detailed explanation on the classification. In Appendix C the data on toxicity are given. When no data are available the average value 3.5 is applied and highlighted in bold. Especially data on reproductive toxicity i.e. endocrine disruption are lacking. The application of the average value (3.5) will be discussed in more detail later.

Of the 137 chemical substances for which data were collected in 1998, toxicity data was only available for 108 substances. Of the 302 substances in the 1999 PRTR, toxicity data was found for all substances.

The unit for emission of dioxins is mg TEQ/year, whereas for all other chemical substances the result is given in kg/year. The dioxins can therefore not be compared with the other chemical substances and are excluded from the ranking. This is unlucky since dioxins are well-investigated chemical substances and extremely toxic. Furthermore, it is unfortunate since dioxins are emitted even though they have been specifically regulated. The regulation only seems to have reduced the emissions by approximately 10%.

The resulting data set for 1998 thus includes 107 chemical substances and for 1999 301 chemical substances for which data on both emissions and toxicity are available in comparable units.

3. Method: Partial order theory and random linear extensions

Partial order theory is a large mathematical discipline and several textbooks are available that cover the topic or related topics, such as Set Theory, Graph Theory, Lattice Theory and Combinatorics (e.g. Birkhoff, 1984; Davey and Priestley, 1990; Bartel, 1996). Basic ideas of partial order theory are further presented in several publications (e.g. Halfon and Reggiani, 1986; Brüggemann and Bartel, 1999; Brüggemann et al., 1999, 2001).

The theory of partial orders has been used to order chemical substances according to their negative effect on human health and the environment (e.g. Halfon and Reggiani, 1986; Brüggemann and Halfon, 1990; Brüggemann and Münzer, 1993; Klein et al., 1995; Galassi et al., 1996; Halfon et al., 1996; Sørensen et al., 1998; Behrendt et al., 1999; Brüggemann and Bartel, 1999; Brüggemann et al., 1999; Lerche et al., 2002a). However, partial order theory has also found uses in relation to other environmental issues.

Partial order theory (POT) is a simple technique that a priori includes "$\leqslant$" as the only mathematical relation (e.g. Davey and Priestley, 1990). Considering a series of chemical substances, which can be described by a set of descriptors (q_j), then a given substance, a, is characterised by the descriptors $q_j(a)$. Another substance, b, is analogously characterised by the descriptors $q_j(b)$. The chemical substances, a and b, can be compared through simultaneous comparison of the individual descriptors. Thus, the substance a will be ranked higher than substance b ($b \leqslant a$) if all descriptors for a are higher than or equal to the corresponding descriptors of b. In mathematical terms this can be expressed as:

$$b \leqslant a \quad \text{if } q_j(b) \leqslant q_j(a) \quad \text{for all } j$$

However, in the special case that all descriptors for a are equal to the corresponding descriptors for b, $q_j(a) = q_j(b)$ for all j, the two objects will have an identical rank and are considered as equivalent, $a \sim b$. In mathematical terms this can be expressed as:

$$a \leqslant b \quad \text{and} \quad b \geqslant a \Longleftrightarrow a \sim b$$

Equivalent objects can be referred to as members of an equivalent class. For a more rigorous introduction of

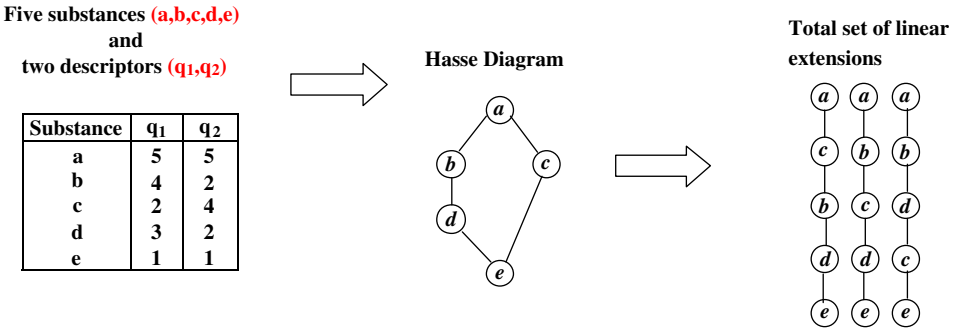
equivalence relations within partial order theory see also Brüggemann and Bartel (1999).

It further follows that if $b \leqslant a$ and $c \leqslant b$ then $c \leqslant a$. If two chemical substances cannot be given an order, they are said to be incomparable (an incomparability).

A partial order can be illustrated in a so-called Hasse diagram (Hasse, 1952), where the connecting lines are drawn between comparable chemical substances. To illustrate the principle a simple Hasse diagram is constructed in Fig. 1 where five fictive chemical substances (a, b, c, d, e) are ranked using two descriptors (q_1, q_2). In Fig. 1 it can be seen that e.g. a is ranked above all other chemical substances since the descriptors for a ($q_1(a) = 5$ and $q_2(a) = 5$) are higher than or equal to the descriptors of all other substances ($q_1(a) \geqslant q_1(x)$ and $q_2(a) \geqslant q_2(x)$, where x is an arbitrary substance). In Fig. 1 substance b and c are incomparable since the first descriptor is larger for b than for c ($q_1(b) = 4 > q_1(c) = 2$) whereas the second descriptor is larger for c than for b ($q_2(c) = 4 > q_2(b) = 2$). It is thus not possible to establish a mutual order between b and c.

The descriptors used in this study are the emission and transfer categories and data on toxicity given in Appendices A–C and in Tables 1 and 2. Note that the descriptors are kept completely separated thus e.g. emission to air is only compared with emission to air. No assumptions are made e.g. if emission to soil is more problematic or costly than emission to air. Further, notice that if a descriptor is added with a profile similar to a descriptor that is already applied, this does not influence the ranking result. Since the POT ranking is a non-metric method, it is the contrast among the descriptors that direct the ranking more than the actual metric values. When a Hasse diagram is constructed normally a chemical substance is placed as high as possible. In this way a kind of precautionary approach is applied. The Hasse diagram thus forms a number of levels. For example in Fig. 1 the Hasse diagram has four levels corresponding to the longest chain (a, b, d, e). The levels in a Hasse diagram can be regarded as a kind of classification (Brüggemann and Steinberg, 2000), where each level indicates a level of environmental impact.

Apart from the choice of descriptors, the only subjective element in POT is the choice concerning classification. Classification generally leads to a simplification of a data set. Since the data on toxicology is grouped into six classes, to facilitate the analysis, the values on production, use and emissions are also organised in six equidistant classes, i.e. the range of each descriptor is divided into six classes of the same equidistant size. This is, however, an arbitrary choice. If no classification is used the analyses of the data are troubled with a large portion of incomparable substances. However, considering the data in the PRTR database most of the descriptors for the chemical substances are classified in either the highest (6) or the lowest class (1) when six



Ranking frequency from the total set of linear extensions

Rank	Substances				
	a	*b*	*c*	*d*	*e*
5	3	0	0	0	0
4	0	2	1	0	0
3	0	1	1	1	0
2	0	0	1	2	0
1	0	0	0	0	3

Ordinal ranking probabilities and the average ranks

Rank	Substances				
	a	*b*	*c*	*d*	*e*
5	1	0	0	0	0
4	0	0.67	0.33	0	0
3	0	0.33	0.33	0.33	0
2	0	0	0.33	0.67	0
1	0	0	0	0	1
Average	5	3.67	3	2.33	1

Fig. 1. The principle of Hasse diagram technique (Lerche et al., 2002a).

classes are applied. This is due to the fact that some chemicals have extremely high emissions to one media in relation to the other chemical substances. It could be argued that the analysis becomes less detailed in this way. However, it is possible to make a more detailed analysis on the chemicals with lower emissions by excluding the high emission chemicals from the analysis.

A linear extension (LE) is a linear rank or a linear order, where all the ordering done in the partial order is preserved (e.g. Davey and Priestley, 1990). A non-trivial partial order can be reproduced in several linear orders. The number of possible linear order increases dramatically with the number of incomparable chemical substances included in the partial order. If all possible linear extensions are found a ranking probabilities, $p_r(i,k)$, for the individual chemical substances, i, can be retrieved for each rank, k. The number of linear extensions where a selected substance has obtained a specific rank relative to the total number of linear extensions is equal to the ranking probability. The principle is illustrated in Fig. 1. The substance a is related to the highest rank only since a is placed above all other chemical substances in all linear extensions. On the other hand, substance c is equally related to three ranking levels. Therefore for substance c the ranking probability for rank nos. 4, 3 and 2 are all equal to 0.33.

Considering the ranking probabilities for all objects on all ranking positions the average rank for a substance can be calculated (Graham, 1982; Winkler, 1982, 1983). The average rank is simply the average of the ranks in all the linear extensions. The average rank for a substance (i) is calculated by summing the multiplication of each rank (k) by its probability (p_r):

$$\mathrm{AverageRank}(i) = \sum_{k=1}^{k=N} k \cdot p_r(i,k)$$

where N is the number of substances. If we use Fig. 1 as an example, the average rank of the substance b is 3.667. For the substance c the average rank is 3. Thus in a random linear extension substance b will most probably be given a higher rank than c. In the example given in Fig. 1 the average rank is thus: $a > b > c > d > e$.

The total number of possible linear extensions is related to the number of incomparable chemical substances. Since the number of incomparable substances will increase with the number of substances if the descriptors are independent, following the combinatorial rule, the upper bound of the number of linear extensions will tend to depend on the faculty of the number of chemical substances. Therefore it is virtually impossible to identify all possible linear extensions for large Hasse diagrams, even using a very large computer. However, recently a method has been developed using a randomly selected fraction of all possible linear extensions (Sørensen et al., 2001; Lerche and Sørensen, 2003; Lerche et al., 2003). The challenge in making random linear extensions is that in order to make a random linear extension without a systematic error the mutual probabilities must be known. The mutual probability is found by only considering two substances at a time. The mutual probability is then the probability that e.g. the first substance is ranked higher than the other substance. Thus, taking into account that when a random linear extensions is created the substances are continuously given mutual ranks, it is advantageous to apply the correct mutual probability. However, in order to calculate the mutual ranking probability all linear extensions must be known. This creates a chicken and egg situation. However there are several ways to make very good estimates of the mutual probabilities (Brüggemann et al., 2002; Lerche et al., 2003). Applying the estimated mutual probabilities have improved the creation of random linear extensions and the method predicts the ranking probabilities within the random uncertainty (Lerche et al., 2003).

4. Results and discussion

If a ranking is desired that is related to specific protection aims the descriptors should be carefully selected according to that protection aim. However, in this study we simply apply all information available in order to obtain a "general" ranking of the chemical substances.

4.1. The 1998 PRTR Hasse diagram based on both emission and toxicity data

The Hasse diagram based on the 1998 PRTR is presented in Fig. 2. This diagram has been produced using the WHASSE computer program (Brüggemann and Halfon, 1995). Due to the large number of substances the diagram may look complicated. However the diagram reveals seven levels. In the top level 33 chemical substances are found. Of these 33 chemical substances, 14 appear to be incomparable with any other substance. These chemical substances are per definition placed in the top level, even though it is not immediately clear if they exhibit environmental impact higher than the chemical substances in the lower levels. The top 19 chemical substances, which are comparable with at least one other substance and thus "qualify" as top chemical substances are: acrylamide (2), acrylonitrile (5), vinyl chloride (17), cadmium compounds (19), chromium compounds (hexavalent) (24), chloropicrin (28), cobalt compounds (34), diazinon (39), 1,4-dichlorobenzene (49), mercury compounds (62), arsenic compounds (87), parathion (89), beryllium compounds (99), benzene (100), dichlorvos (112), ethanol amine (121), ethylben-

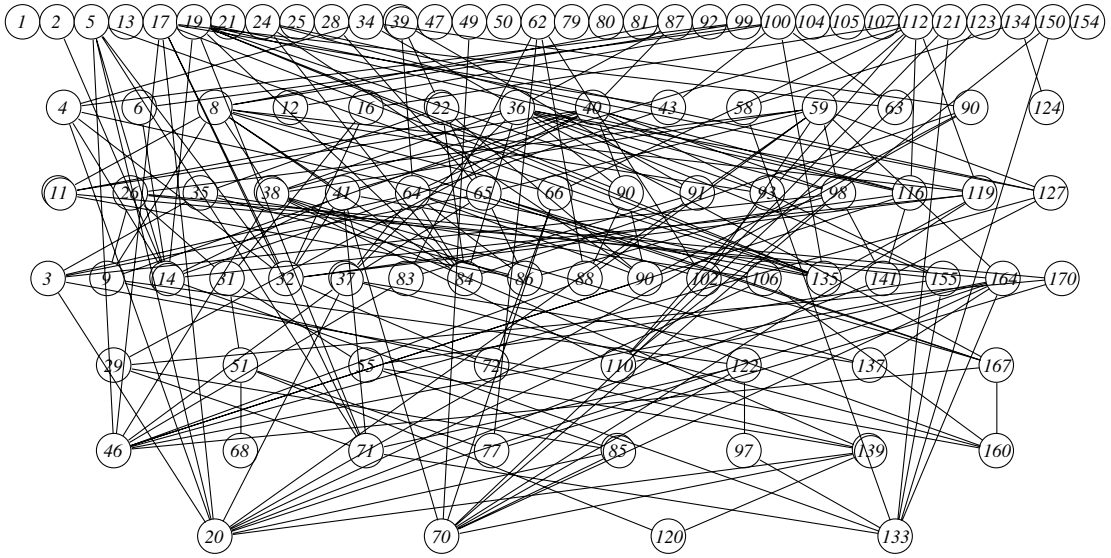


Fig. 2. The Hasse diagram based on the complete 1998 PRTR data set and using mean toxicological values for the missing data. The following substances are ranked equally and only the first substance is shown in the figure: {11;67} {14;42} {22;101} {37;117} {38;108} {39;89} {85;114} and {139;153}.

zene (123), 2-ethoxyethyl acetate (134) and terephthalic acid (150).

4.2. The 1999 PRTR Hasse diagram based on both emission and toxicity data

Since the descriptors, i.e. the emission categories, the number of chemicals included and the geographic area of the 1998 and 1999 PRTR are different it does not make sense to compare the two PRTRs directly.

The Hasse diagram for the PRTR data from 1999 including 301 chemical substances appears to be rather complex due to the large number of substances and is therefore not included in this paper. However, 12 levels can be identified and the top level comprises 38 chemical substances.

4.3. The 1998 PRTR Hasse diagram based on toxicity data only

The Hasse diagram for the 1998 PRTR data based only on the toxicity data has, as a consequence of the application of fewer descriptors, a significant reduction in the number of incomparable chemical substances. Thus, only one substance is found to be incomparable with any other substance and eight levels are identified. The diagram itself is just as complicated as the one in Fig. 2 and is therefore not pictured. However the top level consists of 11 "qualified" chemical substances. These are: acrylamide (2), acrylonitrile (5), cadmium compounds (19), chromium compounds (24 and 25), cobalt compounds (34), diazinon (39), mercury compounds (62), arsenic compounds (87), lead compounds (80), parathion (89), beryllium compounds (99) and dichlorvos (112). All chemical substances found in the top level are also found in the top level of the Hasse diagram of Fig. 2. In the Hasse diagram based only on the toxicity data, mainly the metals obtain high rankings. This is due to the fact that the metals are well investigated and that based on the toxicological tests performed they have obtained relative high scores (generally $\geqslant 4$).

4.4. The 1998 PRTR Hasse diagram based on emission data only

In the Hasse diagram based on the 1998 PRTR data on emission, transfer, use and production alone there are no chemical substances which is not ordered with respect to at least one other substance. However only five levels are identified. The lower number of levels is probably due to the lower number of equivalent classes and the lower number of equivalent classes is mainly caused by a large group of chemical substances, which only usage is as pesticides. The top level includes 13 chemical substances: zinc compounds (1), acrylonitrile (5), xylene (21), 1,3-dochloropropene (47), 1,4-dichlorobenzene (49), dichloromethane (50), toluene (79), nickel compounds (81), benzene (100), formaldehyde (105), manganese compounds (107), ethanol amine (121) and nitrobenzene (154). All chemical substances found in the top level are

also found in the top level of the Hasse diagram of Fig. 2. Only acrylonitrile (5) appears to be in the top level of both the Hasse diagram based on emission, transfer, production volume and usage and of the Hasse diagram based on toxicity data.

4.5. The importance of the descriptors for the 1998 PRTR data

In partial order theory it is possible to evaluate the quantitative importance of the applied descriptors (Brüggemann and Halfon, 1995; Brüggemann and Bartel, 1999; Brüggemann et al., 2001). This is done by using the so-called W-matrix, which is a dissimilarity-matrix that assesses the differences of Hasse diagrams. The W-matrix measures the Hamming distance among subset of substances. The Hamming distance is the symmetric difference between any two sets. Thus, for each objects the "down-set", i.e. the objects below, are registered and the differences between these "down-sets" in the partial orders are compared, summed and given in the W-matrix. Thus if one descriptor is excluded and the partial order is compared with the original partial order based on the full set of descriptors a large number in the W-matrix indicates that the descriptor, which was excluded, has a large influence on the structure of the original Hasse diagram.

Thus by excluding the descriptors for the 1998 PRTR one at a time the W-matrix is calculated and given in Table 3. It can be noted that the data on production volume clearly display the major influence on the structure of the Hasse diagram for the 1998 PRTR data. It is interesting to note that the three descriptors on emissions having the highest influence on the structure of the ranking, namely production volume, use and recycling are not used as descriptors in the 1999 survey.

4.6. Ranking probabilities of the 1998 PRTR data

In Fig. 3 the ranking probabilities for the 1998 PRTR are illustrated. Each line corresponds to the ranking probability for one substance. For illustration only five chemical substances, dichlorvos (112), beryllium compounds (99), diphenylmethane-4,4′-disisocyanate (36), dimethoate (139) and 1,1,1-trichloromethane (70) have been accentuated. Considering the ranking probabilities it is interesting to note that if the probability range for one chemical is relative narrow as is the case for diphenylmethane-4,4′-disisocyanate (36) relative to dimethoate (139) this indicate that the estimation of the rank for the first chemical is more certain. Note also that the "noisy structure" of the ranking probabilities is a consequence of the kind of approximative methodology.

Table 3
The importance of the descriptors

Descriptors for emission	W-matrix
Production volume	7428
Usage volume	390
Transfer to recycling	95
Emission due to transportation	23
Transfer to sewage	22
Emission from households and offices	10
Emission due to use as pesticide	8
Emission to water	6
Transfer to waste	1
Emission to air	1
Emission from non-regulated industry	1
Disperse waste	1
Transfer to landfill	0
Emission to soil	0
Descriptor for toxicity	
Aquatic ecotoxicity	532
Cancer	472
Inhalation toxicity	362
Chronic oral toxicity	236
Mutagenecity	176
Allergy	91
Reproductive disorder	79

The number of additional comparabilities in the Hasse diagram in Fig. 2 when the individual descriptors are removed.

4.7. The 1998 PRTR average rank based on both emission and toxicity data

The average rank for the 1998 PRTR is given in Table 4. The top 10 chemical substances, which are expected to exhibit the highest environmental impacts are: dichlorvos (112), inorganic arsenic compounds (87), cobalt compounds (34), beryllium compounds (99), fenitrothion (59), disulfoton (40), parathion (89), diazinon (39), 4,4′-diamino-3,3′-dichlorodiphenylmethane (36) and antimony compounds (8). It is interesting to note that acrylonitrile (5), which was both in the top level of the Hasse diagram based on toxicity data only and emissions data only is not in the top 10 of the final rank. This is probably due to the fact that there is only nine compounds below it in the Hasse diagram. Dichlorvos, fenitrothion, parathion, diazinon and disulfoton are all pesticides containing organic phosphor. Dichlorvos gets its high position because of the high emission due to use as a pesticide combined with a relative high toxicity. Dichlorvos is mainly used as a pesticide for growing vegetables, including potatoes, fruit and tea plants. inorganic arsenic, cobalt, beryllium and antimony compounds are heavy metals, which are used in industrial processes. 4,4′-diamino-3,3′-dichlorodiphenylmethane is a plasticizer used in the hardening of epoxy resins.

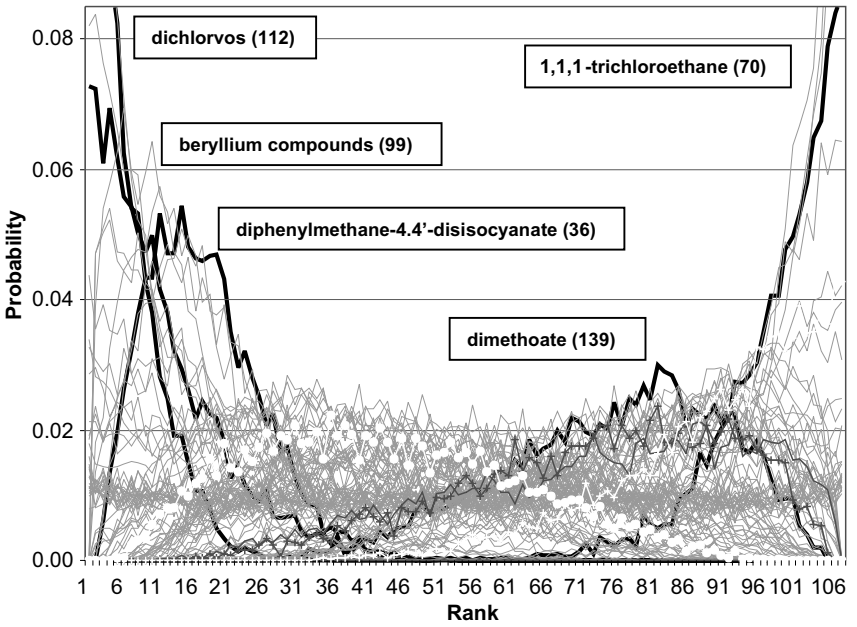


Fig. 3. The ranking probabilities for the chemical substances in the 1998 PRTR.

Apart from fenetrothion (59), disulfoton (40), 4,4′-diamino-3,3′-dichlorodiphenylmethane (36) and antimony compounds (8), the chemical substances ranked as top 10 are all members of the top level in the Hasse diagram (Fig. 2). Fenitrothion (59) is placed in the second level, just below dichlorvos (112), estimated to have the highest environmental impact. Disulfoton (40), 4,4′-diamino-3,3′-dichlorodiphenylmethane (36) and antimony compounds are also placed in the second level both just below arsenic compounds (87). Hence, even if a substance is not located in the top level of the Hasse diagram it might still obtain a high position in the average rank. This is the case if a substance displayed in a Hasse diagram is located immediately below a substance in the top level and at the same time above more chemical substances than other substances in the top level.

4.8. The 1999 PRTR average rank based on both emission and toxicity data

The top 10 chemical substances from the 1999 PRTR are given in Table 5. These are PCBs, lead compounds, fenitrothion, dichlorvos, disulfoton, inorganic arsenic compounds, chlorothalonil, thiobencarb, chromium and HCFC-141b. Only 4 of the top 10 from 1998 can be found among the top 10 from the 1999 PRTR (fenitrothion, dichlorvos, disulfoton and inorganic arsenic compounds). The PCBs get the highest rank due to its high emission to water and transfer as solid waste combined with high toxicity. In 1973 Japan was the first country in the world to prohibit the production and use of PCBs. However, the present emission to waste occurs during storage and destruction of the PCBs. Lead compounds get their high position due to high transfer to landfill and as solid waste and a high toxicity. Thiobencarb and chlorothalonil both have high emissions as pesticides and high aquatic toxicity. As shown in Tables 1 and 2 other substances such as xylene, toluene and manganese all have very high emissions. However, considering the Hasse diagram or the average rank these substances are not among the highest placed ones. This is due to the fact that they have a lower toxicity and therefore these substances only have a limited number of substances below them in the partial order and as such they do not obtain a high position in the Hasse diagram or the average rank. It could be argued that this is a limitation of the POT/RLE methodology. This can be further investigated by analysis of so-called subdiagrams, where it is clear how many substances are actually below a substance of initial interest. Further, other POT-approaches such as the population of event spaces might be considered in order to get an overview of the situation (Lerche, 2003 and references herein).

Both in the top 10 of the 1998 PRTR and the 1999 PRTR there are three groups: pesticides (dichlorvos, fenitrothion, parathion, diazinon, disulfoton, chlorothalonil, thiobencarb), heavy metals (arsenic, cobalt, beryllium, lead, arsenic, antimony and chromium compounds) and industrial chemicals (4,4′-diamino-3,3′-dichlorodiphenylmethane, PCBs and HCFC-141b).

Table 4
The ranking result of the 1998 PRTR

Pilot no.	Name of compound	Average rank	Linear rank
112	Dichlorvos	101.3	107
87	Arsenic compounds	100.7	106
34	Cobalt compounds	97.7	105
99	Beryllium compounds	96.3	104
59	Fenitrothion	96.3	103
40	Disulfoton	92.7	102
89	Parathion	90.9	101
39	Diazinon	90.8	100
36	4,4′-Diamino-3,3′-dichlorodiphenylmethane	90.0	99
8	Antimony compounds	89.0	98
26	Chloropyrifosmethyl	88.1	97
19	Cadmium compounds	87.0	96
100	Benzene	83.0	95
16	Chlorothalonil	82.9	94
17	Vinyl chloride	78.9	93
24	Chromium compounds (hexavalent)	78.7	92
28	Chloropicrin	77.7	91
62	Mercury compounds	76.3	90
101	Benzoepin	74.5	89
22	Silver compounds	74.4	88
134	2-Ethoxyethyl acetate	73.3	87
31	Thiobencarb	70.8	86
5	Acrylonitrile	70.6	85
170	Methidathion	70.1	84
64	Selenium compounds	69.7	83
9	Isoxathion	66.3	82
155	Nonylphenol	65.4	81
4	Ethyl acrylate	65.0	80
41	Carbon tetrachloride	64.4	79
90	(*o*,*p*,*m*)Phenylenediamene	63.1	78
2	Acrylamide	62.8	77
11	Indium compounds	61.3	76
67	Tellurium compounds	61.2	75
119	Isoprene	61.1	74
98	Propoxur	60.6	73
38	Isoprothiolane	60.0	72
108	Fenobucarb	59.5	71
121	Ethanol amine	59.1	70
65	Chlorpyrifos	58.9	69
150	Terephthalic acid	58.4	68
90	(*o*,*p*,*m*)Phenylenediamene	57.7	67
66	Tetrachloroethylene	56.7	66
6	Acetaldehyde	56.3	65
51	Diquat	56.2	64
49	1,4-Dichlorobenzene	55.9	63
123	Ethylbenzene	55.8	62
35	Fenbutatin oxide	55.6	61
29	Simazine	55.3	60
116	Aniline	54.7	59
79	Toluene	54.1	58
91	Fenthion	53.7	57
107	Manganese compounds	53.3	56
1	Zinc compounds	53.3	55
105	Formaldehyde	53.2	54
81	Nickel compounds	53.1	53
21	Xylene (mixed isomers)	53.1	52
80	Lead compounds	52.9	51
47	1,3-Dichloropropene	52.8	50
13	Epichlorohydrin	52.8	49
154	Nitrobenzene	52.8	48
50	Dichloromethane	52.7	47
104	Boron compounds	52.7	46
55	Diphenylmethane-4,4′-diisocyanate	52.6	45
92	1,3-Butadiene	52.4	44
122	Molinate	52.2	43
25	Chromium compounds (except hexavalent)	52.0	42
43	1,2-Dichloroethane	51.6	41
127	Cabaryl	50.7	40
93	DEHP	50.1	39
12	Ethylene oxide	46.2	38
102	Pentachloronitrobenzene	46.1	37
58	Dimethylformamide	45.0	36
124	2-Ethoxyethanol	44.2	35
164	1,6-Hexanediamine	43.3	34
63	Styrene	42.1	33
37	Cyanide compounds	38.9	32
117	Allyl alcohol	38.9	31
88	Hydrazine	35.4	30
106	Malathion	34.7	29
68	Copper compounds	34.6	28
97	Propyzamide	34.1	27
83	Thiram	34.1	26
139	Dimethoate	32.0	25
153	Nitrotoluenes	31.9	24
3	Acrylic acid	30.7	23
114	Bis(2-ethylhexyl) adipate	30.5	22
77	Trifluraline	30.2	21
32	Chloroform	30.1	20
85	Paraquat	30.0	19
167	Mancozeb	29.9	18
84	Vanadium compounds (divanadium pentaoxide)	29.5	17
90	(*o*,*p*,*m*)Phenylenediamene	29.6	16
141	Biphenyl	27.5	15
71	1,1,2-Trichloroethane	25.6	14
135	Vinyl acetate	24.7	13
86	Barium compounds	23.2	12
42	1,4-Dioxane	22.6	11
14	1,2-Epoxypropane	22.5	10
72	Trichloroethylene	18.4	9
110	Molybdenum compounds	18.3	8
137	2,4-D	17.3	7
120	Bisphenol A	17.2	6
160	Dibutyl phthalate	11.5	5
70	1,1,1-Trichloroethane	8.8	4
46	1,2-Dichloropropane	7.5	3
133	Chloromethane	6.6	2
20	Caprolactam	5.9	1

Table 5
The top 10 ranking from the 1999 PRTR

CAS no.	PRTR number	Name of compounds	Average rank	Linear rank
122-14-5	192	Fenitrothion	256.60	302
62-73-7	350	Dichlorvos	247.33	300
1897-45-6	199	Chlorothalonil	247.08	299
–	230	Lead compounds	245.23	298
119-12-0	186	Pyridaphenthion	242.96	297
1336-36-3	306	PCBs	238.31	296
2636-26-2	184	Cyanophos	236.78	295
2597-03-7	173	Phenthoate	235.03	294
298-04-4	151	Disulfoton	233.81	293
1717-00-6	132	HCFC-141b	233.48	292

It could be argued that it is not possible to rank all three types of chemical substances together (pesticides, heavy metals and industrial chemicals). However, if it is desired the three types of chemical substances could easily be ranked independently giving three ranking lists. However, the chemical substances getting top positions in the overall Hasse diagram and average ranks would also receive the highest positions in "local" diagrams and average ranks.

As mentioned in the introduction a linear rank can also be established using other types of MCAs, such as the addition of the descriptors forming a score. However especially when the number of substances is high the scores tend to aggregate. This is illustrated in Fig. 4a and b, where the aggregation of the 1998 and 1999 PRTR data, respectively, are shown. From the figures it can be verified that the more substances are included, as is the case for the 1999 PRTR data, the more the scores accumulate around a particular score (24.5 in Fig. 4b).

The outlyers identified in Fig. 4a are xylene (21) and toluene (79). Toluene is also identified as an outlyer in Fig. 4b at a score of 48.5. This further indicates that if the aggregation of the descriptors had been used to establish the linear rank, those chemicals with the highest emission had simply been selected.

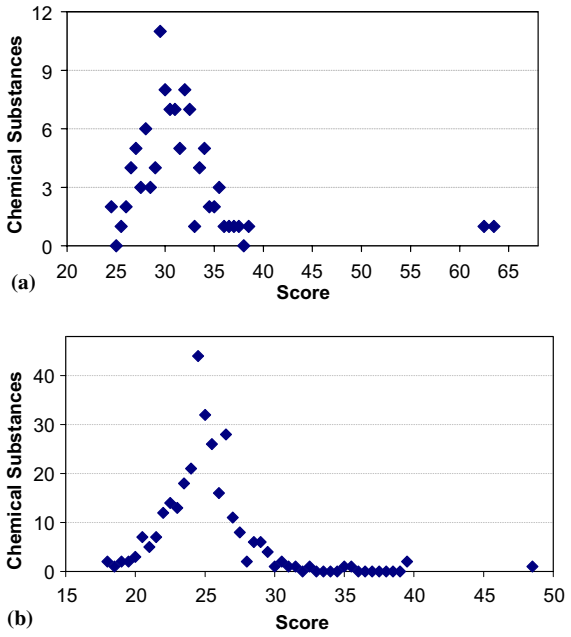


Fig. 4. The distribution of the scores, based on aggregation of the descriptors, for the 1998 PRTR data (a) and the 1999 PRTR data (b).

4.9. Substitution of the missing toxicity data in the 1998 PRTR

As mentioned the data on toxicity are not complete. Some data are missing. It could then be argued that more research should be performed in order to create the missing data or that at least estimates should be made before the ranking analysis could be performed. However, considering the time and cost these investigation would demand it is desirable to find another solution. In this study the possibility of substituting all missing data with the same value is applied.

In the first place the missing data on toxicity were substituted with the mean value of the data set (3.5). This would to some extent imply that the fact that data on toxicity are missing expresses that these chemical substances are not presently subject for major concern, otherwise the toxicity data would have been produced. However, it would on the other hand not be a safe approach to use the value 0 for the missing values and thus rank a dangerous substance low just because the hazards of the substance is unknown. Replacing the missing toxicity data with the mean value is thus a compromise. See Table 6. This substitution will indirectly cause the chemical substances, which are more toxic than the mean, but not yet investigated, to be ranked lower than if they had actually been investigated. In the same way

Table 6
The "no data impact" on the ranking

Type of substitution	Ranking result
Maximum values	"Precautionary approach"
Minimum values	"No uncertainty approach"
Mean values	Compromise

chemical substances which are less toxic than the mean, but not yet investigated, to be given a higher rank than if they had been investigated.

Using a more precautionary approach, the missing values could have been substituted with the maximum values. In this case the non-investigated chemicals would tend to be ranked high and this would motivate the investigation of the chemicals by the producer in the sense that investigation would perhaps provide the chemical with a lower rank. The difference between the rank obtained with missing values substituted with the mean and maximum values respectively would further express how the substitution influences the ranking. If there is are large difference between the two ranks it means that the substitution is crucial for the ranking result.

If a minimum of uncertainty is desired the missing values should be substituted with a the minimum value (1). Then only the substances where information is available and where the values of toxicity are high would get a high score.

It should be noted that when a linear rank is applied and a choice is made concerning the type of substitution, a choice is made on which type of chemical substances that will get a high rank. However, it should be kept in mind that at the same time a choice is made on which chemicals are given a lower rank.

In this study the substitution of the missing data with the maximum value is further investigated. Substituting the missing values with maximum values the resulting Hasse diagram based on all descriptors has nine levels and in the top level there are 23 chemical substances, of which 11 are comparable with at least one other substance. Of these chemical substances there are three chemical substances, which were not in the top level when using mean values for missing values. These are acetaldehyde (6) and indium compounds (11) and tellurium compounds (67). Acetaldehyde gets it high position since the three of the four toxicological values that have been determined are all relative high and in combination with the substitution of the blank with maximum values this overrules the low value for aquatic ecotoxicology (see Appendix C). The indium compounds and the tellurium compounds get their high position since only values for one descriptor is available and it has the maximum value. Consequently, indium and tellurium compounds will have maximum values for all the descriptors on toxicity.

If a Hasse diagram is drawn only based on the descriptors on toxicology and the missing values are substituted with maximum values, then there is only two substances in the top level, indium compounds (11) and tellurium compounds (67). Investigation of the toxicity of indium compounds and tellurium compounds thus appears to be especially needed.

If the average rank is calculated when the missing values are substituted by maximum values, the top 10 chemical substances comprise: tellurium compounds (67), indium compounds (11), chloropyrifosmethyl (26), nonylphenol (155), thiobencarb (31), 4,4′-diamino-3,3′-dichlorodiphenylmethane (36), methidathion (170), disulfoton (40), 1,6-hexanediamine (164) and fenitrothion (59). Of these 10 chemical substances only 4,4′-diamino-3,3′-dichlorodiphenylmethane, disulfoton and fenitrothion were also in the top 10 when using mean values. If the average rank is calculated only using the toxicological descriptors and substituting the missing values with maximum values, the top 10 chemical substances include: indium compounds (11), tellurium compounds (67), nonylphenol (155), disulfoton (40), molinate (122), propyzamide (97), chloropyrifosmethyl (26), isoxathion (9), 4,4′-diamino-3,3′-dichlorodiphenylmethane (36), isoprene (119). Of these 10 chemical substances only disulfoton and 4,4′-diamino-3,3′-dichlorodiphenylmethane were on the list if the average rank is found only for the toxicity data where the missing values are substituted with mean values. The disagreement between the ranking with the missing values substituted with mean and maximum values, respectively, strongly indicates a general need for further toxicological investigations.

4.10. Ranking versus risk assessment

In contrast to conventional risk assessments ranking of chemical substances does not provide a quantitative estimation of the actual risk, it only deals with the relative potential of risk. However, often ranking can be achieved for more chemical substances since lack of and thus exclusion of descriptors e.g. physico-chemical data or biodegradation do not hamper the ranking exercise in the same degree as in the quantitative risk assessment.

The prediction of environmental concentrations (PEC) by fate modelling with the EUSES software (European Commission, 1996) and the ChemCAN (Mackay et al., 1996) have been performed for 68 chemical substances from the 1998 PRTR pilot project (Kawamoto et al., 2001). This study revealed that the predicted environmental concentrations based on the PRTR data were lower than the actual concentration

observed in the environment (Japan Environmental Agency, 1995–1997). This might be due to incomplete PRTR data. However since the calculation was based only on a minor area in Japan, input from other areas could also be expected. However, it remains complicated to verify if the PRTR is complete i.e. if the facilities in the inventory do actually report all their emissions correctly.

The chemical having the highest environmental exposure can be compared with the highest ranked chemicals of the ranking based on emission and transfer data. Using model calculation the substances with the highest emissions were toluene (79) and xylene (21) to air, dimethylformamide (58) and ethanol amine (121) in water and diethylhexylphthalate (93) and dibutylphthalate (160) in the sediment (Kawamoto et al., 2001). Only three of these substances namely toluene (79), xylene (21) and ethanolamine (121) were found in the top level of the Hasse diagram based on emission data only. However since the observed range of concentrations in the environment is very wide, sometimes several orders of magnitude, it is hard to draw any conclusions on the comparisons of the ranking and the modelling results.

Further, the ranking is inherently dependent on the individual descriptors included. It is therefore important that the descriptors are chosen so that they describe the physical, chemical or biological properties relevant for evaluating the impact on environment and human health or in this case, more specifically, the concentrations in the environment. Unfortunately, it may often be difficult to obtain data on the descriptors expected to be the most appropriate. Consequently the descriptors actually being available, and still of relevance, are frequently applied. In this study data on emissions, transfer, production and use are included as indicators for the exposure level. However, to develop a more complete picture of the exposure it would have been desirable if e.g. data on biodegradation in the different environmental compartments had also been available.

Additionally, data on bioaccumulation could be added in order to improve the assessment of the exposure. Further, it could be argued that the degree of recycling does not change the level of exposure and that recycling should not be used if estimating the environmental concentrations is the eventual goal. Data on recycling have nevertheless been included as a descriptor in our study in order to favour chemical substances, which are actually being recycled. Similar arguments go for the figures for production volume and use. It can be argued that these data do not have a direct influence on the environmental concentration. However, imagine the situation where a substance is produced and used without any emissions to the environment. For example, 4,4′-diamino-3,3′-dichlorodiphenylmethane (36), which is a top 10 substance, has only usage but no emissions. However, we believe that this situation is not realistic and the production volume and the figures on usage have been included in the calculation of the rank. These considerations may add to explain some of the discrepancy between the modelling and the ranking result.

5. Conclusion

A general average rank has been established for the 1998 and 1999 PRTR in Japan. The top 10 chemical substances in the 1998 PRTR are: dichlorvos, inorganic arsenic compounds, cobalt compounds, beryllium compounds, fenitrothion, disulfoton, parathion, diazinon, 4,4′-diamino-3,3′-dichlorodiphenylmethane and antimony compounds. The top 10 chemical substances from the 1999 PRTR are: PCBs, lead compounds, fenitrothion, dichlorvos, disulfoton, inorganic arsenic compounds, chlorothalonil, thiobencarb, chromium and HCFC-141b. Only four of the top 10 chemical substances are both in the top 10 of the 1998 PRTR and the 1999 PRTR. The chemical substances belong to three groups: pesticides, heavy metals and industrial chemicals.

The quantitative most important descriptor for the 1998 PRTR is the production volume, which, however, is not applied in the 1999 PRTR. Further, the disagreement between the ranking with the lacking toxicity data substituted with mean and maximum values, respectively, strongly indicate a general need for further toxicological investigations. Finally some discrepancy may exist between the ranking and the model estimates, however it is hard to draw any conclusion on the comparison.

Acknowledgements

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Appendix A

The CAS numbers, the names and the emissions from point sources in the pilot PRTR project in Kanagawa and Aichi prefecture. The values are given in kg/year. Only the 107 substances, which are ranked in this study, are reported in the appendix.

Pilot no.	CAS no.	Name of compound	Emission to air	Emission to water	Emission to soil	Transfer to sewage	Transfer to waste	Transfer to landfill	Transfer to recycling
1	–	Zinc compounds	6200	31 200	27	1480	824 000	127 000	1 740 000
2	79-06-1	Acrylamide	535	706	0	0	0	0	904
3	79-10-7	Acrylic acid	838	5	0	0	307	0	60
4	140-88-5	Ethyl acrylate	2300	5	0	0	354	0	878
5	107-13-1	Acrylonitrile	95 900	1630	0	0	528 000	0	45 000
6	75-07-0	Acetaldehyde	5460	992	0	0	0	0	0
8	–	Antimony compounds	249	254	0	0	2620	54	2620
9	18 854-01-8	Isoxathion	0	0	0	0	0	0	0
11	–	Indium compounds	0	0	0	0	210	0	0
12	75-21-8	Ethylene oxide	57 300	19	0	290	0	0	0
13	106-89-8	Epichlorohydrin	2060	2100	0	4	11 900	0	0
14	75-56-9	1,2-Epoxypropane	58 100	22	0	0	0	0	0
16	1897-45-6	Chlorothalonil	0	0	0	0	0	0	0
17	75-01-4	Vinyl chloride	53 400	10	0	0	0	100	0
19	–	Cadmium compounds	26	6	0	0	2510	1400	415 000
20	105-60-2	Caprolactam	403	3	0	1	1100	0	0
21	1330-20-7	Xylene (mixed isomers)	6 720 000	50 000	138	5	980 000	0	1 450 000
22	–	Silver compounds	0	0	0	25	34	0	334
24	–	Chromium compounds (hexavalent)	48	39	0	3	21 200	0	4790
25	–	Chromium compounds (except hexavalent)	40	665	0	43	220 000	30 000	4 570 000
26	5598-13-0	Chloropyrifosmethyl	0	0	0	0	0	0	0
28	776-06-2	Chloropicrin	0	0	0	0	0	0	0
29	122-34-9	Simazine	0	0	0	0	0	0	0
31	28 249-77-6	Thiobencarb	0	0	0	0	0	0	0
32	67-66-3	Chloroform	1970	7	0	416	15 700	0	990
34	–	Cobalt compounds	64	472	0	0	1280	0	12 800
35	13 356-08-6	Fenbutatin oxide	0	0	0	0	0	0	0
36	101-14-4	4,4′-Diamino-3,3′-dichlorodiphenylmethane	0	0	0	0	0	0	0
37	–	Cyanide compounds	2180	350	0	39	7930	0	2050
38	50 512-35-1	Isoprothiolane	0	0	0	0	0	0	0
39	333-41-5	Diazinon	0	0	0	0	0	0	0
40	298-04-4	Disulfoton	0	0	0	0	0	0	0
41	56-23-5	Carbon tetrachloride	100	0	0	0	129	0	0
42	123-91-1	1,4-Dioxane	33 800	242	0	35	22 200	0	50 200
43	107-06-2	1,2-Dichloroethane	133 000	497	0	0	66 200	0	0
46	78-87-5	1,2-Dichloropropane	7900	4140	0	0	7750	0	0
47	542-75-6	1,3-Dichloropropene	0	0	0	0	0	0	0
49	106-46-7	1,4-Dichlorobenzene	100	400	0	0	0	0	0
50	75-09-2	Dichloromethane	1 440 000	343	11	0	274 000	0	92 500
51	85-00-7	Diquat	0	0	0	0	0	0	0
55	101-68-8	Diphenylmethane-4,4′-diisocyanate	18 700	0	0	0	37 400	0	0
58	68-12-2	Dimethylformamide	39 600	1040	0	0	82 900	0	541
59	122-14-5	Fenitrothion	0	0	0	0	0	0	0
62	–	Mercury compounds	13	0	0	0	0	0	0
63	100-42-5	Styrene	101 000	32	0	0	11 100	0	3860
64	–	Selenium compounds	498	0	0	0	0	0	0
65	2921-88-2	Chlorpyrifos	0	0	0	0	0	0	0
66	127-18-4	Tetrachloroethylene	33 100	22	0	995	13 800	0	4850
67	–	Tellurium compounds	22	6	0	0	311	0	0

Appendix A (*continued*)

Pilot no.	CAS no.	Name of compound	Emission to air	Emission to water	Emission to soil	Transfer to sewage	Transfer to waste	Transfer to landfill	Transfer to recycling
68	–	Copper compounds	4	733	1	152	142 000	0	216 000
70	71-55-6	1,1,1-Trichloroethane	12 700	30	0	0	1470	0	6960
71	79-00-5	1,1,2-Trichloroethane	474	5	0	0	0	0	0
72	79-01-6	Trichloroethylene	123 000	1320	0	0	60 200	0	133 000
77	1582-09-8	Trifluralin	0	0	0	0	0	0	0
79	108-88-3	Toluene	7 330 000	6010	221	5750	1 220 000	0	810 000
80	–	Lead compounds	444	725	0	11	193 000	1400	1 750 000
81	–	Nickel compounds	270	18 900	7	218	115 000	249 000	987 000
83	137-26-8	Thiram	0	0	0	0	309	0	0
84	1314-62-1	Vanadium compounds (divanadium pentaoxide)	7	318	0	0	16 500	9500	260 000
85	1910-42-5	Paraquat	0	0	0	0	0	0	0
86	–	Barium compounds	0	3640	0	0	16 300	0	15 500
87	–	Arsenic compounds	18	169	0	7	22 600	0	111
88	302-01-2	Hydrazine	288	3030	0	57	2300	26	0
89	2104-64-5	Parathion (EPN)	0	0	0	0	0	0	0
90	95-54-5/106-50-3/108-45-2	(*o*,*p*,*m*)Phenylenediamene	0	0	0	0	26	0	1390
90	95-54-5/106-50-3/108-45-2	(*o*,*p*,*m*)Phenylenediamene	0	0	0	0	26	0	1390
90	95-54-5/106-50-3/108-45-2	(*o*,*p*,*m*)Phenylenediamene	0	0	0	0	26	0	1390
91	55-38-9	Fenthion	0	0	0	0	0	0	0
92	106-99-0	1,3-Butadiene	432 000	779	0	0	7750	0	1 330 000
93	117-81-7	DEHP	23 700	10	0	0	22 600	0	57 500
97	23 950-58-5	Propyzamide	0	0	0	0	0	0	0
98	114-26-1	Propoxur	0	0	0	0	0	0	0
99	–	Beryllium compounds	0	0	0	0	0	0	23
100	71-43-2	Benzene	336 000	950	1	0	384	0	34
101	115-29-7	Benzoepin	0	0	0	0	0	0	0
102	82-68-8	Pentachloronitrobenzene	0	0	0	0	0	0	0
104	–	Boron compounds	1510	36 400	0	8300	180 000	12 400	20 000
105	50-00-0	Formaldehyde	55 100	4690	0	6	36 300	39 900	653
106	121-75-5	Malathion	0	0	0	0	0	0	0
107	–	Manganese compounds	491	4390	0	7	292 000	0	1 160 000
108	3766-81-2	Fenobucarb	0	0	0	0	0	0	0
110	–	Molybdenum compounds	286	336	13	390	19 800	30 500	151 000
112	62-73-3	Dichlorvos	34	0	0	0	0	0	0
114	103-23-1	Bis(2-ethylhexyl) adipate	0	0	0	0	56	0	2970
116	62-53-3	Aniline	100	0	0	0	0	0	0
117	107-18-6	Allyl alcohol	111	940	0	0	60	0	0
119	78-79-5	Isoprene	20 800	0	0	0	710	0	8000
120	80-05-7	Bisphenol A	0	53	0	0	837	0	1140
121	141-43-5	Ethanol amine	328	28 600	0	19 000	42 600	0	0
122	2212-67-1	Molinate	0	0	0	0	0	0	0
123	100-41-4	Ethylbenzene	9830	2	0	0	354	0	0
124	110-80-5	2-Ethoxyethanol	109 000	0	0	0	21 000	0	2020
127	63-25-2	Cabaryl	0	0	0	0	0	0	0
133	74-87-3	Chloromethane	220 000	1850	0	0	0	0	0
134	111-15-9	2-Ethoxyethyl acetate	56 500	0	0	0	4120	0	23 900

(*continued on next page*)

Appendix A (*continued*)

Pilot no.	CAS no.	Name of compound	Emission to air	Emission to water	Emission to soil	Transfer to sewage	Transfer to waste	Transfer to landfill	Transfer to recycling
135	108-05-4	Vinyl acetate	61 600	168	0	0	170	0	1150
137	94-75-7	2,4-D	0	0	0	0	0	0	0
139	60-51-5	Dimethoate	0	0	0	0	0	0	0
141	92-52-4	Biphenyl	95	0	0	0	0	0	0
150	100-21-0	Terephthalic acid	3	0	0	0	364	0	0
153	25 321-14-6	Nitrotoluenes	0	0	0	0	27 400	0	0
154	98-95-3	Nitrobenzene	200	219 000	0	0	0	0	0
155	25 154-52-3	Nonylphenol	0	0	0	0	49	0	0
160	84-74-2	Dibutyl phthalate	0	0	0	0	1480	0	784
164	124-09-4	1,6-Hexanediamine	0	0	0	0	0	0	0
167	07-01-18	Mancozeb	0	0	0	0	0	0	0
170	950-37-8	Methidathion	0	0	0	0	0	0	0

Appendix B

The production, use and the emissions from diffuse sources in the pilot PRTR project in Kanagawa and Aichi prefecture. The values are given in kg/year. Only the 107 substances, which are ranked in this study, are reported in the appendix.

Pilot no.	Production volume	Usage volume	Emission due to use as pesticide	Emission due to transportation	Emission from households and offices	Emission from non-regulated industry	Disperse waste
1	2 270 000	11 300 000	123	0	0	0	267 000
2	37 900 000	1 090 000	0	0	1	2	0
3	0	4 960 000	0	0	0	0	0
4	0	3 920 000	0	0	0	0	0
5	1 990 00 000	59 700 000	0	0	12	16	0
6	174 000	1 230 000	0	94 700	0	0	0
8	0	394 000	0	0	0	0	0
9	0	0	4740	0	0	0	0
11	1000	2500	0	0	0	0	0
12	2 480 00 000	40 300 000	0	0	0	0	0
13	19 100 000	127 000	0	0	0	0	0
14	20 100 000	7 190 000	0	0	0	0	0
16	0	0	6010	0	0	0	0
17	94 900 000	1 180 00 000	0	0	0	0	0
19	51 800	2 730 000	0	0	0	0	0
20	1 100 00 000	1 230 000	0	0	0	0	0
21	7 950 00 000	4 660 00 000	0	201 000	836 000	1 130 000	0
22	1850	7070	0	0	0	0	0
24	10 800	416 000	0	0	0	0	0
25	275	6 860 000	0	0	0	0	0
26	0	0	208	0	0	0	0
28	1 530 000	0	48 300	0	0	0	0
29	0	0	960	0	0	0	0
31	0	0	8920	0	0	0	0
32	0	40 300	0	0	4150	0	0
34	134 000	474 000	0	0	0	0	0
35	0	0	154	0	0	0	0
36	0	12 800	0	0	0	0	0
37	43 200 000	35 500 000	1050	0	0	0	0
38	0	0	6130	0	0	0	0
39	16 000	0	7060	0	0	0	0

Appendix B (*continued*)

Pilot no.	Production volume	Usage volume	Emission due to use as pesticide	Emission due to transportation	Emission from households and offices	Emission from non-regulated industry	Disperse waste
40	0	0	6410	0	0	0	0
41	0	349	0	0	0	0	0
42	23 600	117 000	0	0	0	0	0
43	1 150 00 000	85 500 000	0	0	0	0	0
46	2 880 000	51 200	0	0	0	0	0
47	0	0	135 000	0	0	0	0
49	29 500	3500	0	0	694 000	0	0
50	170 000	2 610 000	0	0	0	0	0
51	0	0	4510	0	0	0	0
55	0	3 240 000	0	0	0	0	0
58	87 400	735 000	0	0	0	0	0
59	0	0	12 400	0	0	0	0
62	0	0	0	0	0	0	93
63	665 000	84 400 000	0	0	3500	4590	0
64	0	837	0	0	0	0	0
65	0	0	697	0	0	0	0
66	0	915 000	0	0	0	0	0
67	0	17 800	0	0	0	0	0
68	263 000	1 550 000	5460	0	0	0	0
70	9 800 000	17 100	0	0	0	0	0
71	1 830 000	0	0	0	0	0	0
72	0	12 900 000	0	0	0	0	0
77	0	0	3400	0	0	0	0
79	7 180 00 000	3 430 00 000	0	183 000	757 000	1 060 000	0
80	466 000	21 400 000	0	0	0	0	0
81	10 200	2 290 000	0	0	0	0	0
83	0	4180	1800	0	0	0	0
84	31 000	335 000	0	0	0	0	0
85	0	0	1880	0	0	0	0
86	1710	340 000	0	0	0	0	0
87	21 000	20 500	0	0	0	0	0
88	0	74 200	0	0	0	0	0
89	0	0	2190	0	0	0	0
90	0	132 000	0	0	0	0	0
90	0	132 000	0	0	0	0	0
90	0	132 000	0	0	0	0	0
91	0	0	3080	0	0	0	0
92	1 680 00 000	1 300 00 000	0	26 200	0	0	0
93	60 600 000	3 530 000	0	0	0	0	0
97	0	0	594	0	0	0	0
98	0	0	320	0	0	0	0
99	0	469	0	0	0	0	0
100	2 910 00 000	1 750 00 000	0	125 000	0	39 800	0
101	0	0	1310	0	0	0	0
102	0	0	1890	0	0	0	0
104	2540	2 480 000	0	0	0	0	0
105	85 100	9 250 000	0	227 000	87 900	6420	0
106	0	0	2550	0	0	0	0
107	1 470 000	7 100 000	0	0	0	0	144 000
108	0	0	6440	0	0	0	0
110	0	1 780 000	0	0	0	0	0
112	1000	34	12 800	0	0	0	0
114	0	126 000	0	0	0	0	0
116	0	45 600	0	0	0	0	0
117	0	14 100 000	0	0	0	0	0

(*continued on next page*)

Appendix B (*continued*)

Pilot no.	Production volume	Usage volume	Emission due to use as pesticide	Emission due to transportation	Emission from households and offices	Emission from non-regulated industry	Disperse waste
119	0	5 910 000	0	0	0	0	0
120	74 200 000	15 300 000	0	0	0	0	0
121	11 700 000	1 440 000	0	0	14 400	0	0
122	0	0	1580	0	0	0	0
123	70 300 000	22 700 000	0	46 400	527	691	0
124	3 570 000	3 290 000	0	0	11 700	15 400	0
127	0	0	2560	0	0	0	0
133	0	145 000	0	0	0	0	0
134	0	644 000	0	0	13 100	17 100	0
135	0	6 140 000	0	0	2610	1490	0
137	0	0	1130	0	0	0	0
139	0	0	1950	0	0	0	0
141	2 890 000	20 000	0	0	0	0	0
150	2 860 00 000	1 290 00 000	0	0	0	0	0
153	45 800	0	0	0	0	0	0
154	0	238 000	0	0	0	0	0
155	0	861 000	0	0	0	0	0
160	0	80 600	0	0	2860	3750	0
164	0	190 000	0	0	0	0	0
167	0	0	15 300	0	0	0	0
170	0	0	5070	0	0	0	0

Appendix C

The toxicity data for the national PRTR project. The values are distributed in six classes. Only the 107 substances, which are ranked in this study, are reported. The bold region indicates that no data were available. These missing values have been filled in by a mean value (3.5).

Pilot no.	Chronic oral toxicity	Inhalation toxicity	Cancer	Reproductivty	Mutagenecity	Allergy	Aquatic ecotoxicity
1	1	5	2	**3.5**	**3.5**	**3.5**	5
2	5	6	4	**3.5**	3	**3.5**	1
3	1	5	2	**3.5**	**3.5**	**3.5**	5
4	**3.5**	3	4	**3.5**	3	4	4
5	6	4	4	**3.5**	3	**3.5**	4
6	**3.5**	4	4	**3.5**	3	**3.5**	1
8	4	6	4	**3.5**	**3.5**	**3.5**	4
9	4	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	4
11	**3.5**	6	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**
12	**3.5**	4	5	**3.5**	3	3	1
13	5	5	4	**3.5**	3	3	2
14	**3.5**	3	4	**3.5**	3	**3.5**	1
16	3	**3.5**	4	**3.5**	**3.5**	**3.5**	6
17	4	4	5	**3.5**	3	**3.5**	**3.5**
19	4	6	5	4	3	**3.5**	6
20	1	3	2	**3.5**	3	**3.5**	**3.5**
21	2	2	2	**3.5**	**3.5**	**3.5**	4
22	3	6	2	**3.5**	**3.5**	**3.5**	6
24	3	6	5	**3.5**	3	4	6
25	3	5	5	**3.5**	**3.5**	4	5
26	4	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	6
28	**3.5**	5	2	**3.5**	**3.5**	**3.5**	6
29	4	**3.5**	3	**3.5**	**3.5**	**3.5**	5
31	3	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	6
32	3	3	4	**3.5**	3	**3.5**	3

Appendix C (*continued*)

Pilot no.	Chronic oral toxicity	Inhalation toxicity	Cancer	Reproductivty	Mutagenecity	Allergy	Aquatic ecotoxicity
34	**3.5**	6	4	**3.5**	**3.5**	4	5
35	2	6	2	**3.5**	**3.5**	**3.5**	6
36	**3.5**	6	4	**3.5**	**3.5**	**3.5**	5
37	3	4	2	**3.5**	**3.5**	**3.5**	5
38	3	4	**3.5**	**3.5**	**3.5**	**3.5**	4
39	4	6	2	**3.5**	**3.5**	**3.5**	6
40	4	6	**3.5**	**3.5**	**3.5**	**3.5**	5
41	4	3	4	**3.5**	**3.5**	**3.5**	3
42	**3.5**	3	4	**3.5**	3	**3.5**	1
43	4	3	4	**3.5**	3	**3.5**	1
46	3	4	2	**3.5**	3	3	**3.5**
47	4	3	4	**3.5**	3	3	5
49	2	2	4	**3.5**	**3.5**	**3.5**	4
50	3	2	4	**3.5**	3	**3.5**	1
51	3	**3.5**	**3.5**	**3.5**	**3.5**	3	6
55	3	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	5
58	**3.5**	3	3	4	**3.5**	**3.5**	1
59	4	5	**3.5**	**3.5**	**3.5**	**3.5**	6
62	5	5	3	**3.5**	**3.5**	3	6
63	3	2	4	**3.5**	3	**3.5**	2
64	4	6	2	**3.5**	**3.5**	**3.5**	5
65	3	5	2	**3.5**	**3.5**	**3.5**	6
66	4	2	4	**3.5**	**3.5**	**3.5**	4
67	**3.5**	6	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**
68	1	**3.5**	**3.5**	**3.5**	**3.5**	3	6
70	2	1	3	**3.5**	**3.5**	**3.5**	3
71	4	3	3	**3.5**	3	**3.5**	3
72	3	2	4	**3.5**	3	**3.5**	3
77	3	**3.5**	3	**3.5**	**3.5**	3	6
79	2	2	2	**3.5**	**3.5**	**3.5**	4
80	4	5	4	5	**3.5**	**3.5**	5
81	3	6	5	**3.5**	**3.5**	4	**3.5**
83	4	5	2	**3.5**	3	3	6
84	3	6	2	3	3	**3.5**	4
85	3	**3.5**	3	**3.5**	**3.5**	**3.5**	5
86	2	5	2	**3.5**	**3.5**	**3.5**	3
87	4	6	5	**3.5**	**3.5**	**3.5**	5
88	**3.5**	4	3	**3.5**	3	3	5
89	4	6	2	**3.5**	**3.5**	**3.5**	6
90	**3.5**	6	3	**3.5**	3	3	5
90	**3.5**	6	2	**3.5**	3	4	5
90	3	6	2	**3.5**	3	3	5
91	4	5	2	**3.5**	3	**3.5**	6
92	**3.5**	4	4	**3.5**	3	**3.5**	**3.5**
93	3	4	4	**3.5**	**3.5**	**3.5**	2
97	4	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	1
98	2	5	3	**3.5**	**3.5**	**3.5**	5
99	4	6	5	**3.5**	**3.5**	4	4
100	4	4	5	**3.5**	3	**3.5**	2
101	3	6	2	**3.5**	**3.5**	**3.5**	6
102	4	5	2	**3.5**	**3.5**	3	5
104	2	5	**3.5**	**3.5**	**3.5**	**3.5**	1
105	2	5	4	**3.5**	3	4	2
106	2	4	2	**3.5**	**3.5**	**3.5**	6
107	2	5	2	**3.5**	**3.5**	**3.5**	5
108	3	4	**3.5**	**3.5**	**3.5**	**3.5**	4
110	3	4	**3.5**	**3.5**	**3.5**	**3.5**	1

(*continued on next page*)

Appendix C (*continued*)

Pilot no.	Chronic oral toxicity	Inhalation toxicity	Cancer	Reproductivty	Mutagenecity	Allergy	Aquatic ecotoxicity
112	4	5	4	**3.5**	**3.5**	**3.5**	6
114	3	**3.5**	3	**3.5**	**3.5**	**3.5**	5
116	3	5	4	**3.5**	3	**3.5**	5
117	3	4	2	**3.5**	**3.5**	**3.5**	5
119	**3.5**	**3.5**	4	**3.5**	**3.5**	**3.5**	3
120	2	**3.5**	**3.5**	**3.5**	**3.5**	3	4
121	**3.5**	4	**3.5**	**3.5**	**3.5**	**3.5**	1
122	4	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	3
123	2	2	4	**3.5**	**3.5**	**3.5**	4
124	**3.5**	2	**3.5**	4	**3.5**	**3.5**	1
127	3	4	3	**3.5**	3	**3.5**	6
133	**3.5**	3	3	**3.5**	3	**3.5**	1
134	**3.5**	3	**3.5**	4	**3.5**	**3.5**	2
135	**3.5**	2	4	**3.5**	3	**3.5**	2
137	3	4	2	**3.5**	**3.5**	**3.5**	3
139	3	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	4
141	1	4	3	**3.5**	3	**3.5**	5
150	**3.5**	4	**3.5**	**3.5**	**3.5**	**3.5**	1
153	3	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	4
154	3	4	4	3	**3.5**	**3.5**	4
155	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**	5
160	1	4	2	**3.5**	**3.5**	3	4
164	**3.5**	4	**3.5**	**3.5**	**3.5**	**3.5**	**3.5**
167	3	5	2	**3.5**	**3.5**	3	4
170	4	**3.5**	3	**3.5**	**3.5**	**3.5**	6

Appendix D

List of abbreviations.

CFC	Chlorofluorocarbon
HCFC	Hydrochlorofluorocarbon
LE	Linear extensions
OECD	Organisation for Economic Co-operation and Development
PCB	Polychlorobiphenyls
PEC	Predicted environmental concentration
POT	Partial order theory
PRTR	Pollutant Release and Transfer Register
RLE	Random linear extensions
UNCED	United Nations Conference on Environment and Development
UN-ECE	United Nation Economic Commission for Europe
TEQ	Toxic equivalent
MCA	Multi-criteria analysis

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