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AN IMPROVED RANKING SCHEME FOR ENVIRONMENTAL HAZARDS

by

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ABSTRACT

The partial ordering ranking scheme developed in 1985 has been extended to include data uncertainties and a number of standard chemicals. This formal approach ranks chemicals for environmental hazard according to test results relevant to their fate and/or toxicity using a vectorial approach. In this paper we examine two interesting case studies. The inclusion of uncertainty in the Hasse diagram and a new procedure to include standards in the Hasse diagram so that the ranking scheme does not change when additional chemicals are added. The proposed method allows one to visually compare chemicals based on a large number of test results which might otherwise be very confusing when displayed in a Table form: The Hasse diagram is an effective graphical display of data difficult to understand otherwise.

RESUME

Le système de classement par ordre d'importance établi en 1985 a été élargi de manière à inclure les données incertaines et un certain nombre de produits chimiques standard. Avec cette approche formelle, on classe les substances chimiques en fonction de leur nocivité pour l'environnement selon les résultats des essais qui se rapportent à leur évolution ou à leur toxicité en utilisant une méthode vectorielle. Dans cet article, nous examinons deux intéressantes études de cas. L'inclusion de l'incertitude dans le diagramme de Hasse de sorte que le système de classement ne change pas lorsqu'on ajoute d'autres produits chimiques. La méthode proposée permet de comparer visuellement les produits chimiques à partir d'un grand nombre de résultats d'essais qui, autrement, pourraient être très embrouillants s'ils étaient présentés sous forme de tableau : le diagramme de Hasse est une présentation graphique efficace de données qui seraient difficiles à comprendre autrement.

PERSPECTIVE DE GESTION

Le système de classement par ordre d'importance établi en 1985 a été élargi de manière à inclure les données incertaines et un certain nombre de produits chimiques standard. Avec cette approche formelle, on classe les substances chimiques en fonction de leur nocivité pour l'environnement en se basant sur les résultats des essais qui se rapportent à leur évolution et à leur toxicité en utilisant une méthode vectorielle. La méthode proposée permet de comparer visuellement les dangers que représentent les produits chimiques pour l'environnement à partir d'un grand nombre de résultats d'essais. L'analyse des mêmes résultats d'essais pourraient, autrement, être très embrouillante quand les données sont présentées sous forme de tableau : le diagramme de Hasse est une présentation graphique efficace de données qui seraient difficiles à comprendre autrement. De plus, la méthode repère les résultats d'essais qui pourraient être en contradiction avec ceux d'autres tests et par conséquent tient compte des incertitudes dans le classement par ordre d'importance. Ailleurs, cette méthode a également été adoptée pour classer les pesticides par ordre d'importance.

MANAGEMENT PERSPECTIVE

The partial ordering ranking scheme developed in 1985 has been extended to include data uncertainties and a number of standard chemicals. This formal approach ranks chemicals for environmental hazard according to test results relevant to their fate and/or toxicity using a vectorial approach. The proposed method allows one to visually compare the hazard posed by chemicals to the environment based on a large number of tests results. The analysis of the same test results might otherwise be very confusing when data are displayed in a Table form: The Hasse diagram is an effective graphical display of data difficult to understand otherwise. The method also identifies test results which might contradict results from other tests and therefore introduce uncertainty in the ranking. Elsewhere this method has also been applied to rank pesticides.

INTRODUCTION

Ranking chemicals in terms of their environmental hazard by prespecified criteria, has been the subject of much research (1,2,3,4). In this paper we expand on a formal procedure, based on set theory and systems analysis, developed a few years ago (5) to rank chemicals, using the information available from a variety of degradation and fate tests, and to analyze the data.

Partial ordering is a vectorial approach which recognizes that not all chemicals can be directly compared with all other chemicals in terms of environmental hazard when several criteria are used. In fact, the higher the number of criteria used, the higher the probability that contradictions exist between the criteria so that different ranking results might originate. With the approach presented here, contradictions are solved in a holistic way using decision theory. Results are displayed on paper or on a TV monitor driven by a desk top personal computer using Hasse diagrams (6,7), a useful graphic tool commonly used in algebra to display lattices (a genealogical tree is a special case of a Hasse diagram). This method not only ranks chemicals but also identifies contradictions in the criteria used to rank the chemicals. Analysis of the data used in the ranking scheme is an important part of the ranking scheme itself. In a Hasse diagram (8) the chemicals closer to the bottom of the figure are the least hazardous. The numbers in each circle are labelled (Table 1) and the lines between the circles mean that the given chemicals can be directly compared with each other following any path. By definition, the chemicals on the same level are "incomparable" (see example in Fig. 1b and explanation in the theory section for definition of incomparability).

The method stated here is based on the hypothesis that a set of numbers is generally necessary to create a ranking file; these numbers can be considered the elements of a vector, the "vector performance" or "vector distance". This

"vector approach method" is different from the "scalar approach method", where a single number (a scalar performance index) is said to be sufficient to interpret fate and toxicity data and to compare chemicals and rank them according to their environmental hazard. The main point is that rather than inventing new methods of decision making, i.e. to develop new indices, we make a more realistic contribution by using existing methods borrowed from another field of science to classify and evaluate real chemicals using large data sets. The basic premise of this ranking scheme is that a low numerical value on a test indicates less environmental hazard. Therefore, if for some tests the opposite premise is valid, i.e., a high numerical value means less environmental hazard, then the ranking must be inverted by multiplying all values by -1. For example, a high degradation rate indicates less environmental hazard and therefore the reciprocal or the negative of any rate is used as an element of the vector distance with the assumption that the lower the value of an element of the vector distance, the lower the environmental hazard. In fact high values of bioaccumulation indicate possible environmental hazard whereas high degradation rates indicate less environmental hazard.

THEORY

For each chemical, a given number of tests, called attributes, is performed. Once several attributes are chosen the next step is to assign them weighting factors. This step can be left to the expert (9) and can be included or bypassed in the vectorial procedure; initially in this presentation all attributes are assumed to have equal importance but later a procedure to include weighting factors is also presented. The assumption of equal weights is valid if, before the vectorial analysis is performed, we check the set of attributes for completeness; i.e. if the set is adequate and contains enough information

nonredundant (to avoid double counting), to rank the chemicals for environmental hazard).

The number of attributes should be minimal to reduce the number of experiments required for each chemical; this condition implies that the properties of the attributes should be independent of one another. The attributes and their values can be expressed in a simple mathematical form: Each chemical is linked to a set of numbers, each number corresponding to the result of a single test; the numbers so defined are the elements of the vector distance and the ranking is defined in such a way to decrease as the environmental hazard decreases.

The ranking procedure

The formal logical development of the method can be found in (8). A BASIC program to display results with a desk top personal computer is available from the author. The hazard levels are determined by comparing the test data for each chemical with all the others according to prespecified logical rules. These rules are the definition of binary relations between pairs of set elements and are based on principles of lattice and graph theory developed during the 1970's (5-8; 10); the methodology is therefore well established and the procedure is described here with an example. A computer program has been developed for easy usage of the method, but the method is simple enough that calculations can be done also by hand even if they are lengthy.

A set of data is partially ordered if contradictions exist in the test data that prevent us from ranking the contaminants in a chain (Fig. 1a). If contradictions exist for the ranking of two chemicals, then the two chemicals may be assigned to the same hazard level (Fig. 1b) depending also on their relative ranking with the other chemicals in the list.

Two examples

a) Let C1 and C2 be two chemicals and VC1 and VC2 their respective vector distances. If every component of VC1 is lower than the corresponding one of VC2, C1 is obviously the safer of the two. Should any two successive chemicals C2, C3; C3, C4; ... of the considered set {C1, C2, ... } behave in the same fashion we could draw the diagram (Fig. 1a) known in set theory as the Hasse diagram. Here C1 is better than C2; C2 better than C3, and so on. The chemicals can be ranked in a chain. Unfortunately, such a situation, so simple to be understood and sketched, is seldom verified in reality. Consider, for example, the chemical C1 having as components for the vector distance the numbers [4,4] and the chemicals C2 and C3 characterized by the components [2,3] and [3,2]. Both C2 and C3 are better than C1 because they have smaller components than C1. Nevertheless, they are "incomparable" to each other (C2 is better than C3 as far as the first component is concerned, but the opposite is true for the second component (see Fig. 1b). Under these circumstances, it is not immediately apparent which of the two chemicals C2 and C3 is environmentally safer. With a larger number of chemicals and a larger number of tests the ranking becomes even more complicated.

b) In the general case, the formal ranking procedure can be explained by analyzing a small set of data (Table 1): the chemicals are identified as #1; #6; #23; #24; #28; and #34. The Hasse diagram for these six chemicals can be derived as follows: Assume that the six chemicals are positioned at the vertices of a regular polygon, in this case an hexagon (see Fig 2). Now, compare one chemical, e.g. #1 with all others (#6, #23, #24, #28, #34) one at the time. In practice this comparison of chemicals implies the comparison of each individual test (each vector element) performed on one chemical with the respective tests on all the other chemicals, one chemical at the time. In principle, there are four possible

relationships to describe the outcome:

#1 = #6	case A
#1 >/ #6	case B
#1 \< #6	case C
#1 and #6 are incomparable	case D

The notation >/ (greater or equal) of case B) means that each element of chemical #1 is greater or equal than each element of #6, i.e $\#1_1 >/ \#6_1$; $\#1_2 >/ \#6_2$; ... with the constraint that the sign = can not be valid for all elements, since this is case A or the two chemicals occupy the same place in the ranking scheme. If the symbol >/ is interpreted as a parental relation (father-son; father-grandson; grandfather-grandson, etc.) within a family, the Hasse diagram becomes a genealogical tree. The lines represent the direct relation father-son and each two successive levels represent the passage of a generation. For example if we compare each element of #1 with each element of #6 (that is each element on line one in Table 1 with each element in line two) we find that

$\#1_1$ (380) > $\#6_1$ (6);

$\#1_2$ (94) > $\#6_2$ (5.1);

$\#1_3$ (0.1) = $\#6_3$ (0.1);

$\#1_4$ (19) > $\#6_4$ (13);

$\#1_5$ (.30) > $\#6_5$ (.10);

$\#1_6$ (119) > $\#6_6$ (98).

Since each element of #1 is greater than or equal to each respective element of #6, we can draw an oriented line in Fig. 2b from #1 to #6. This example reflects case B. Case C is the the inverse of Case B. If in the present example case C had been true then #6 and #1 would have been connected with an oriented line from #6 to #1, the opposite of case B. If by chance the results of all tests were the same for #6 and #1 then we could say that #1 and #6 rank exactly the same or #1 =

#6 (case A) and graphically the hexagon would then become a pentagon since #1 and #6 would occupy the same space.

Case D is most interesting from the point of view of data analysis. In the Hasse diagram two elements (for example #1 and #23 in Fig 2b) are not connected because contradictions exist among the different tests; these elements are called "incomparable". This contradiction exists also between chemicals #24 and #28. From analysis of Table 1 we see that

$\#24_1$ (2690) < $\#28_1$ (11500);

$\#24_2$ (2420) > $\#28_2$ (2320);

$\#24_3$ (0.1) < $\#28_3$ (39.8);

$\#24_4$ (63) < $\#28_4$ (278);

$\#24_5$ (10) > $\#28_5$ (3.33);

$\#24_6$ (286) > $\#28_6$ (192).

Out of six experiments #24 is less hazardous than #28 (lower numerical value) in three experiments and more hazardous in the other three. Therefore the results are inconclusive and overall we cannot say whether #24 is better than #28 or viceversa. The Hasse diagram (Fig. 2b) identifies #24 and #28 as incomparable by not connecting the two circles; lack of connection identifies contradiction in data. By definition all chemicals located in the same ranking level in a Hasse diagram are incomparable. Similar contradictions exist between #23 and #24 and between #1 and #23. The results of this analysis show that this method is useful not only for ranking but also, and perhaps even more importantly, for data analysis to identify contradictions in the test results.

Continuing the analysis of the example, we compare the pairs #1-#23, #1-#24, #1-#28 and #1-#34 and oriented lines are drawn accordingly following the

Table 1: Vector distance components*: data from Freitag et al.

identification number	name of chemical	algae BF_1 (1)	fish BF_2 (2)	rat % retention (3)	act. sludge BF_5 (4)	act. sludge % CO_2 (5)	% CO_2 (6)
1	toluene	380	94	0.1	19	0.3	119
6	benzoic acid	6	5.1	0.1	13	0.1	98
23	biphenyl	540	280	0.4	26	0.6	105
24	2,2'-dichlorobiphenyl	12690	2420	0.1	63	10.	286
28	2,4,6,2',4'-pentachlorobiphenyl	11500	2320	39.8	278	3.3	192
34	hexachlorobenzene	24800	2600	55.7	350	10.	667

*The first four columns are the relative bioaccumulation rates. The last two columns are the scaled inverse of the degradation rates. Inverse because higher values of degradation are preferable while high bioaccumulation is not. The ranking direction must be the same in absolute terms.

same rules explained in the previous paragraph. The next step is to compare the pairs #6-#23, #6-#24, #6-#28 and #6-#34; and so on until #24-#28; #24-#34 and finally #28-#34. When this analysis is completed, then we have Fig. 2b, or the relation diagram.

The next step is to eliminate all redundant oriented lines. For example the line #34-#23 in Fig. 2b is redundant since the lines #34-#28 and #28-#23 already exist. That is, we know that #23 is less hazardous than #34 since all tests in #23 have numerical values lower than in #34 and all test values of #23 are lower than those of #28 which in turn are lower than those of #34. Therefore, the line between #34 and #23 becomes superfluous since this information already is displayed in the Hasse diagram with the two lines #34-#28 and #28-#23.

Likewise, we can eliminate #28-#6 (the information is contained in #28-#23 and #23-#6); #24-#6; #34-#6 and #34-#1. Figure 2c shows the simplified diagram after all eliminations have been done. The next step is to reorganize the diagram so that the oriented lines are directed towards the bottom of the page (Fig. 2d) so that the arrows become unnecessary. Chemicals of greater environmental hazard are located above those of less hazard. In the final drawing the number of horizontal levels which contain the incomparable elements must be minimized and therefore the chemicals #28 and #24 and the chemicals #23 and #1 are presented in the same level.

As mentioned before we can also introduce the concept of tolerance or weighting factors for each attribute. This option may be necessary when results from laboratory tests have some uncertainty or measurement errors associated with them. For example in test example analyzed above (Table 1) we noted that element $\#24_2$ with a value of 2420 was larger that element $\#28_2$ with a value of 2320. These experimental results are quite similar and if we are

[illegible]

[illegible]

[illegible] illustrated in the Moser diagram with [illegible]

[illegible]

[illegible]

[illegible]

not absolutely sure that the difference is real our interpretation of the results might be flawed. In this example, if we decide that 2320 and 2420 are practically the same, compared for example with other test results of 280 (element #23_2) or 94 (element #1_2), then the solution is to categorize the experimental results into classes. The total range of an attribute is divided, or quantized, into equal or nonequal parts (or categories). In this case, the second vector element of Table 1 can be divided into three arbitrary classes (0-100; 100-1000; 1000-10000). Using this classification scheme elements #24_2 and #28_2 are now equal. From a practical point of view we have added weights to the data. The more confidence we have in the individual test values, the larger the number of classes and viceversa. Thus, an attribute which is divided into few classes (limit case is 2) is given less importance while an attribute which is divided into an infinite number of classes (i.e. we use the raw data), is considered very important.

UNCERTAINTY

The example discussed in the previous section is easily understood and the interpretation of the Hasse diagram (Fig. 2d) is not subject to misunderstandings. Each chemical is ranked at a specific level and the relations between chemicals are clear. The lines connecting the circles indicate the direct comparability of two chemical. To illustrate some problems that might exist when the relations among some chemicals are uncertain we now add two hypothetical chemicals (#10 and #15 in Table 2) to show more complex relationships. When we display a Hasse diagram we can also use one of two conventions.

Convention 1: we give a chemical the benefit of doubt and rank it with minimal risk.

Convention 2: we rank it with maximum risk (worst case situation).

Figure 3 shows the Hasse diagram presented in Fig. 2d with the addition of two hypothetical chemicals #10 and #15 (Table 2) using each of these two conventions. Figure 3a shows the Hasse diagram with the minimal risk (or best case) and Fig. 3b shows the same Hasse diagram with the maximal risk (or worst case). From the analysis of figures 3a and 3b we note that the chemicals #10 and #15 are located in two different positions according to the convention we use. At this stage we have two options. One is to plot the Hasse diagram using always the same convention (for example the worst case), or alternatively we can include the uncertainty of the ranking of chemicals #10 and #15 by plotting the circles not on any specific level but in between the levels identified in Fig. 3a and 3b. The resulting Hasse diagram is then displayed in Fig. 4 where the chemicals with uncertain rank are displayed with a double circle around them. The reader can therefore immediately identify the parts of the Hasse diagram which do not change according to the convention used and parts of the diagram which change. This information might be helpful when real data are analyzed.

Table 2: Vector distance components*: data from Freitag et al. plus two hypothetical compounds to explain the uncertainty principles in Hasse diagrams.

identification number	name of chemical	algae BF_1 (1)	fish BF_2 (2)	rat % retention (3)	act. sludge BF_5 (4)	act. sludge % CO_2 (5)	% CO_2 (6)
1	toluene	380	94	0.1	19	0.3	119
6	benzoic acid	6	5.1	0.1	13	0.1	98
10	chemical A	600	300	1.0	20	1.0	90
15	chemical B	10000	2500	60.0	300	0.8	500
23	biphenyl	540	280	0.4	26	0.6	105
24	2,2'-dichlorobiphenyl	12690	2420	0.1	63	10.	286
28	2,4,6,2',4'-pentachlorobiphenyl	11500	2320	39.8	278	3.3	192
34	hexachlorobenzene	24800	2600	55.7	350	10.	667

*The first four columns are the relative bioaccumulation rates. The last two columns are the scaled inverse of the degradation rates. Inverse because higher values of degradation are preferable while high bioaccumulation is not. The ranking direction must be the same in absolute terms.

ASSIGNMENT OF STANDARDS

The previous paragraph has shown one intrinsic weakness of the partial ordering method, namely the fact that the Hasse diagram might change when new chemicals are added to the list. For example, if we add a chemical that is ranked between #28 and #23, the Hasse diagram might show five levels instead of four and furthermore the levels of #24 and #1 might be become uncertain. These problems can be solved by using a different approach to analyze the available information. As the reader will see, when this approach is used, the levels in the Hasse diagram do not change when additional chemicals are added. This approach is very useful since we have now the possibility of adding standards, well known chemicals, which anyone can refer to when studying new chemicals. Furthermore, when necessary or when new knowledge is obtained, new standards can easily be added. This new Hasse diagram can be described using the same data set employed up to now.

The first step is to divide the data into classes. Using this approach we can not use the raw data any more, but if we are very confident in the data we can decide to use an arbitrary large number of classes; an upper number of 20 classes is suggested. This classification scheme should take into consideration that the

experimental data might contain only information from a limited number of chemicals, or a small set of all possible results. The classes should therefore include all possible results that might be expected if we included all possible chemicals. For example, if we consider the octanol/water partition coefficient, we might create 10 classes, each including chemicals with log K_{ow} in different ranges, for example, 0-1, 1-2, ..., 7-8, ...

If we use the following classes for the six attributes, then Table 2 becomes Table 3:

attribute 1 [0-100; 101-1000; 1001-10000; 10001-20000; 20001-)

attribute 2 [0-100; 101-1000; 1001-)

attribute 3 [0-10; 10.1-)

attribute 4 [0-100; 101-)

attribute 5 [0-1; 1.1 -)

attribute 6 [0-100; 101-300; 301-)

Note that we have divided attribute 1 into five classes, attributes 2 and 6 into 3 classes and attributes 3, 4 and 5 into two classes. Therefore, as explained before, we have added weights to the data; we consider attribute 1 the most important followed by 2 and 6 and finally by 3,4 and 5. Of course other users of the method might disagree and use other weights. If all attributes were divided into the same number of classes, for example three, then all attributes would have the same weight.

The second step in the assignment of standards is to sum the values of the elements for each attribute. This information is included in column 7 in Table 3. This step is equivalent to creating a scalar index.

The third step is to use the information in Table 3 to create a Hasse diagram. The method described in the Theory section can be used to assess the connections between chemicals. The ranking level is assigned by the value in column 7 of Table 3. Figure 5 shows this final Hasse diagram. The vertical position of an individual chemical in this diagram will not change as long as classification does not change. By adding new chemicals only the connectivity of the circles in the Hasse diagram will change. This connectivity map is very important since it includes information about any contradiction of test results.

Table 3: Vector distance components[a]: data from Freitag et al. plus two hypothetical compounds grouped in classes as explained in text.

identification number	name of chemical	algae BF_1 (1)	fish BF_2 (2)	rat % retention (3)	act. sludge BF_5 (4)	act. sludge % CO_2 (5)	% CO_2 (6)	level (score) (7)
1	toluene	2	2	1	1	1	2	9
6	benzoic acid	1	1	1	1	1	1	6
10	chemical A	2	2	1	1	1	1	8
15	chemical B	3	3	2	2	1	3	14
23	biphenyl	2	2	1	1	1	2	9
24	2,2'-dichlorobiphenyl	3	3	1	1	2	2	12
28	2,4,6,2',4'-pentachlorobiphenyl	4	3	2	2	2	2	15
34	hexachlorobenzene	5	3	2	2	2	3	17

[a]The first four columns are the relative bioaccumulation rates. The last two columns are the degradation rates. The inversion used in the previous two table is not used since this information is included in the classification scheme.

DISCUSSION

The proposed method allows one to visually compare chemicals based on a large number of test results which might otherwise be very confusing when displayed in a Table form: The Hasse diagram is an effective graphical display of data difficult to understand otherwise. The truth is that the reality that we wish to represent is difficult to classify and comprehend by the human mind. When reality is simple (elements in a chain) there are no problems of visual display.

The ranking procedure using a vectorial approach is applicable to variety of problems in environmental toxicology. Once data have been collected, a computer can process them in a few seconds. A graphical display program has been developed for desk top computers and is available on request. The number of different classification levels is directly proportional to the number of chemicals and inversely proportional to the number of criteria; in fact the more criteria are considered at the same time, the higher is the probability of contradictions in the data and therefore higher the probability of having fewer discrimination levels.

Hasse diagrams show which chemicals are the most environmentally hazardous. When a new chemical is developed and its properties known, it can be easily ranked and compared with other known chemicals or any arbitrary standards. The availability of the program in microcomputer form make routine application easy.

A final comment: The development of a suitable index for environmental risk has been widely discussed in the literature (3,4,11). An index is a suitable scalar function of the vector distance components with the best chemicals having the lowest index. Since an index is a scalar quantity, problems concerned with the incomparability of chemicals cannot arise since the chemicals can always be ranked and represented as a chain in a Hasse diagram. Unfortunately, ranking chemicals using an index function does not allow the identification of

contradictions in the data as exemplified in this paper. We should be avoiding some procedures that are apparently simpler (scalar indices) because we may run the risk that we gain simplicity by distorting the reality.

REFERENCES

(1) Freitag, D.; Lay, J.P.; Korte, F. In "QSAR in Environmental Toxicology", Kaiser, K.L.E. Ed., D. Reidel Publishing Co.; Dordrecht, 1984; p 111-136.

(2) Kaiser, K.L.E.; Dixon, D.G; Hodson, P.V. In "QSAR in Environmental Toxicology", Kaiser K.L.E. Ed., D. Reidel Publishing Co., Dordrecht and Boston, 1984; p. 189-206.

(3) Klein, W; Geyer, H. Freitag, D.; Rohleder, H. Chemosphere, 1984, 13, 203-211.

(4) Serat, W.F.; Budinger, F.E.; Mueller, P.K. J. Bact., 1965; 90, 832-833.

(5) Halfon, E.; Reggiani, M. Environ. Sci. Technol., 1986, 20,1173-1179.

(6) Preparate, F.P.; Yeh, R.T. "Introduction to discrete structures". Addison-Wesley, Reading, Mass., 1973.

(7) Warfield, J.N. IEEE Trans. Systems Man and Cyber., 1973; SMC-3, 121-132.

(8) Reggiani, M.G.; Marchetti, F.E. IEEE Trans. Systems Man and Cyber., 1975; SMC-5, 322-330.

(9) Keeley, R.L; Raiffa, H. "Decisions with Multiple Objectives": Preferences and Value Tradeoffs". John Wiley & Sons, New York and Toronto, 1976; 400 pp.

(10) Harary, F. "Graph Theory". Addison, Wesley, Reading, Mass., 1969.

(11) Koch, R. In "QSAR in Environmental Toxicology", Kaiser K.L.E. Ed., D. Reidel Publishing Co., Dordrecht and Boston, 1984; p.207-222.

FIGURE LEGENDS

Figure 1. a) Hasse diagram of ranked chemicals C1-C4. C1 is less hazardous than C2, C2 less than C3, etc. b) Hasse diagram of partially ordered chemicals. Both C2 and C3 are better than C1 but they are incomparable with each other. Thus, it is not immediately clear which chemical should be chosen as the safest.

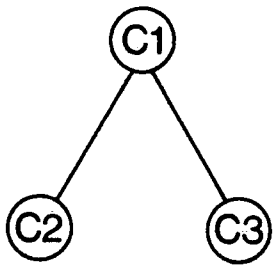
Figure 2. The formal procedure to rank chemicals according to environmental hazard is explained using six chemicals from Table 1. See text for additional explanations. a) set chemicals at vertices of regular polygon. b) rank chemical with one another. c) remove redundant lines d) rotate diagram and eliminate arrows, i.e. Hasse diagram.

Figure 3. The eight chemicals from Table 2 have been ordered according to the two conventions. Figure 3a, minimal risk convention; Figure 3b, maximum risk convention. Circles represent the chemicals and lines indicate that these chemicals can be directly compared. Labels are defined in Table 2. See text for further details.

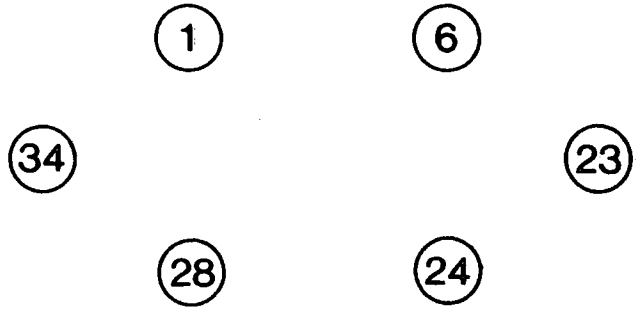
Figure 4. The same eight chemicals shown in Fig. 3 are shown in this Hasse diagram. The two chemicals #10 and #15 occupy a position in between two levels and are marked with double circles to indicate their uncertain rank.

Figure 5. The same eight chlorobenzenes shown in Figures 3 and 4 are ranked according to the criteria shown in Table 3. Note that also information about the total score is used to determine the level in this Hasse diagram.

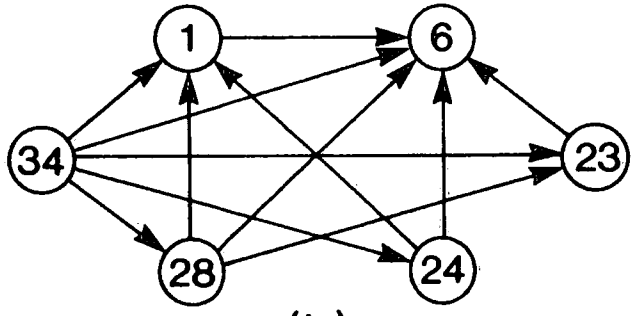
(a)



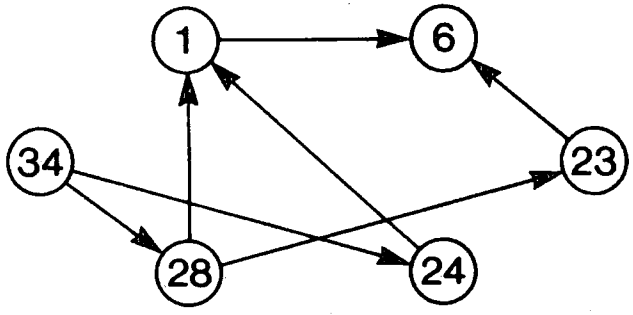
(b)



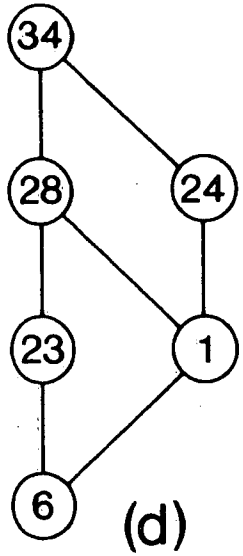
(a)



(b)

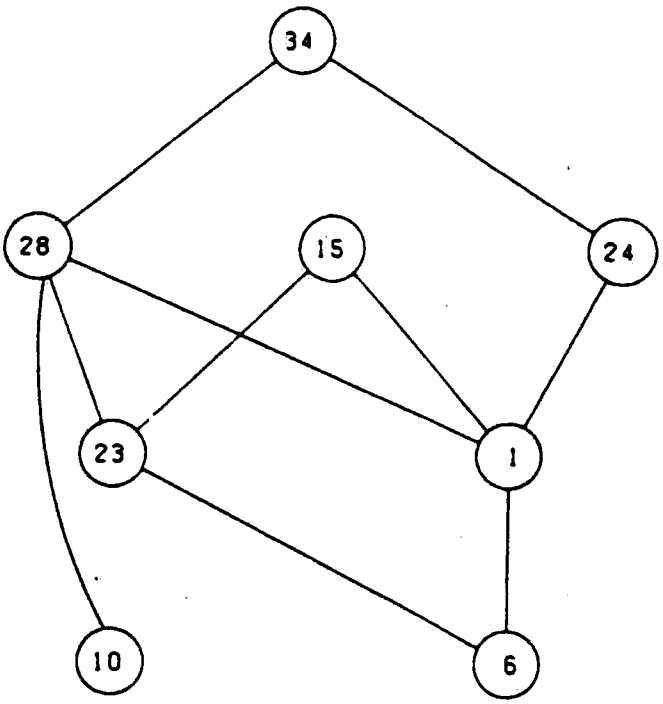


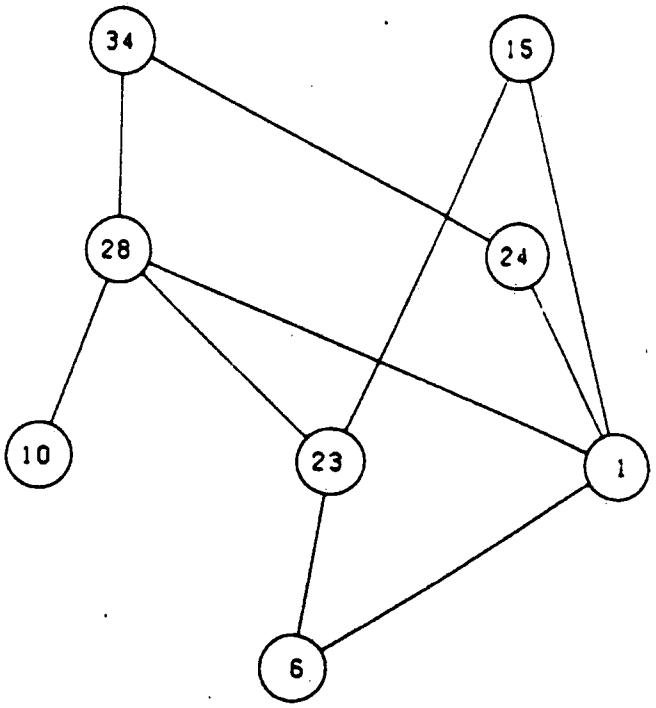
(c)



(d)

More Hazardous

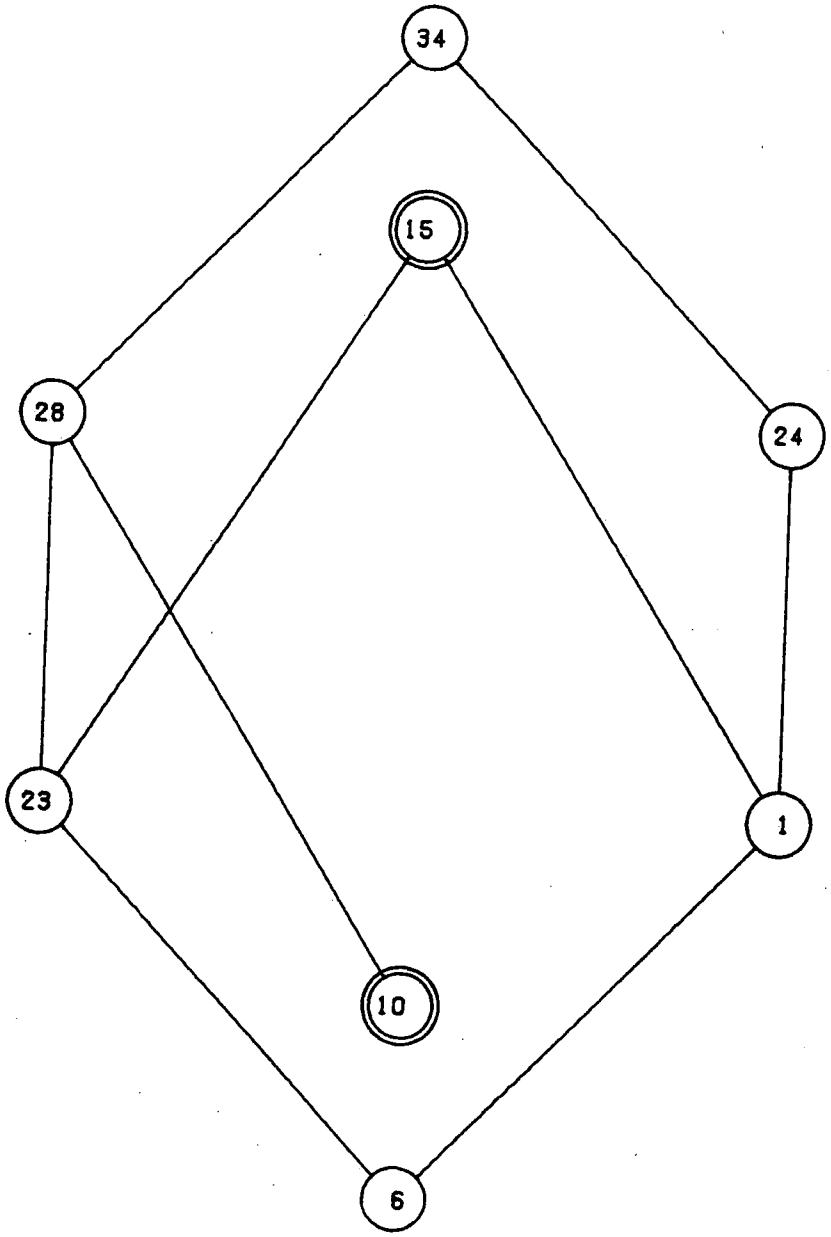




Less Hazardous

(a)

(b)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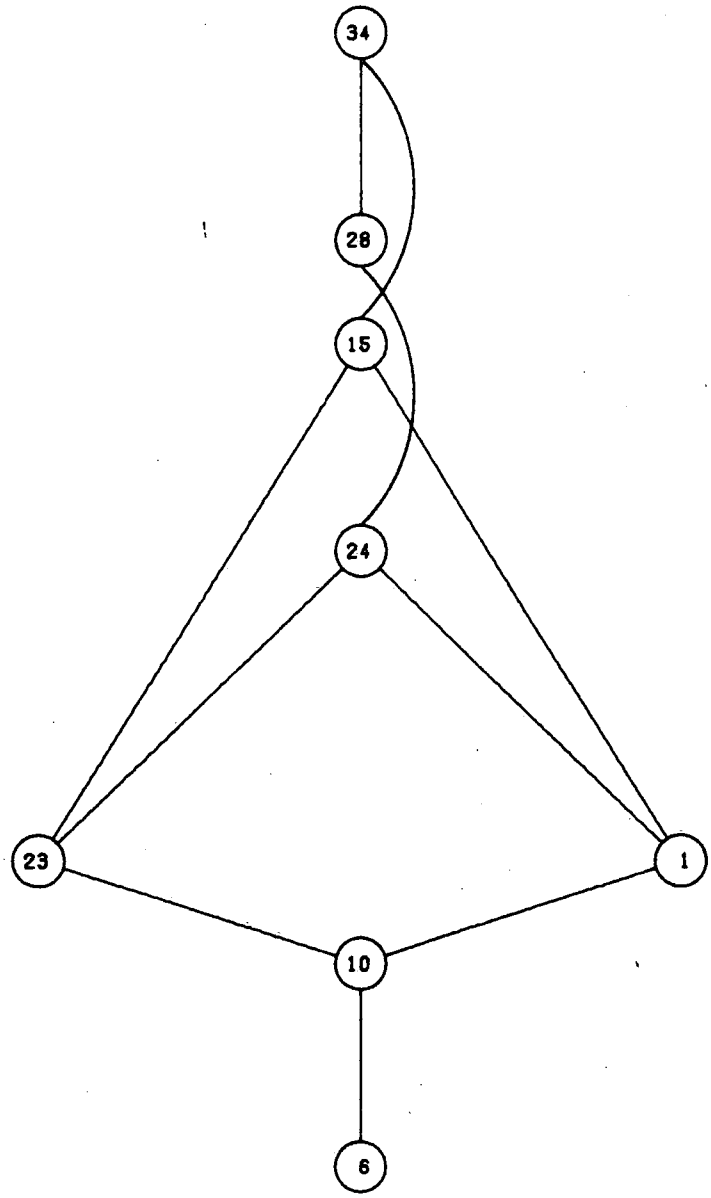
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