A Theoretical Concept To Rank Environmentally Significant Chemicals†

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We assess the environmental hazards of 13 pesticides by means of Hasse diagrams. These diagrams are graph theoretical visualizations of partially ordered sets. A multicriteria assessment is performed, and some methodological aspects are shown. Besides the ranking results there are shown stability, sensitivity, and robustness studies. An EDV-code is available from the first author, which draws the graphs and calculates several characteristic quantities. As evaluative properties the persistence, the aqueous solubility, the vapor pressure, and the yearly usage are taken. It is shown that (i) six pesticides out of 13 are of higher risk, (ii) the selected properties are rather complete to perform a ranking, and (iii) the most important property to rank the chemicals is the aqueous solubility.

INRODUCTION

Ranking of objects, not only of chemicals, is an important first step of risk assessment in environmental sciences. There are many approaches of how to do this; rather elaborated procedures can be found in economics and operations research. As an example the utility function concepts[1,2] should be mentioned, which partially is based on the EDV-code QUALIFLEX, which has its origin in economics.[3] Often—especially in ecosystemic considerations—a deterministic quality function cannot be found. Then the ranking is performed by help of an arbitrary aggregation of information. This means that an object may be characterized by several properties (for example, chemicals by different fate descriptors like geoaccumulation, mobility, etc.) and—lacking causal arguments—the properties will be combined simply operationally. In general simple functions are used. An example may be the GUS-index[4] or a similar concept presented by Fiedler.[5] As Zitko[6] explained, there is no generally accepted method to rank objects.

We will show that there is an alternative way applying basic concepts of the theory of partially ordered sets (posets). The advantage is the strict use of a visualization technique, called the Hasse diagram technique. Hasse diagrams were originally introduced into environmental sciences by Halfon et al.[7,8]

BASIC CONCEPTS

Definitions. The rank of objects is the result of a sequence of comparisons. Therefore the main and crucial step is how to compare objects, which are characterized by many properties; properties which are considered important for the ranking and which often cannot be provided easily.

We call the set of objects P and will denote the elements of P, the objects, by a, b, c, ...x, y. The properties, which have (i) a common orientation (for example: a large value implies a high contribution to a risk) and (ii) an intrinsic importance for the evaluative process are denoted as p_1, p_2, ...,p_i,...,p_n and are called *evaluative properties.* Evaluative properties form a set, the *information base* of evaluation, IB. The quantity $p_i(a)$ is the value of the property p_i of $a \in P$. Each object $x \in P$ is assigned a tuple $p(x) = (p_1(x),...,p_n(x))$ of evaluative properties by a mapping f

$$P \xrightarrow{f} IR^n$$

$$x \mapsto p(x) = (p_1(x),p_2(x),...,p_n(x))$$

IR^n is the set of n-tuples of real numbers, n = card IB ("*card*inality", i.e., the number of elements of IB). Whereas a comparison among objects with $n = 1$ is very easy because this is the natural order of the ray of numbers, a comparison with $n > 1$ is not easy because it is not naturally explained. This is the reason why ranking of multivalued objects is commonly performed after some kind of aggregation "g" which leads to a ranking index, say λ, a scalar

$$P \xrightarrow{f} IR^n \xrightarrow{g} IR$$

$$x \mapsto p(x) \mapsto \lambda$$

The mapping g often is a weighted sum of evaluative properties, and the arbitrariness evolves from the assumptions of the (i) functional form of g and (ii) numerical values of the weights or parameters of g.

When a generalized ordering is wanted, then some additional definitions are needed. The natural order in the one-dimensional case as mentioned above should be included as a specific case. Therefore a general order, "≤" obeys three axioms:

(1) reflexivity $a = a$

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(2) antisymmetry $a \le b$ and $b \le a$, then $a \sim b$.
"$\sim$" denotes an equivalence relation

(3) transitivity $a \le b, b \le c \Rightarrow a \le c$ (1)

"$\le$"-relations obeying these three axioms are called "quasi orderings".

Several remarks should be made:

1. The demands after reflexivity or irreflexivity, antisymmetry or symmetry, or after transitivity, etc. lead to a whole class of algebraic relations among objects. (An order theoretical consideration of binary algebraic relations was performed by Ganter.[9]) For example, if instead of antisymmetry, symmetry is demanded, then the algebraic binary relation of equivalence follows.

2. The demand for antisymmetry can be sharpened to

$$a \le b \quad \text{and} \quad b \le a \quad \Longrightarrow \quad a = b$$

Then—instead of quasi ordering—a partial ordering arises

3. There are many realizations of ordering. For example the divisor relation on natural numbers is a partial order; another example is the inclusion of sets or the logical "imply-relation".

Here the realization of the quasi ordering, which is suitable for ranking is as follows:

$$a,b \in P$$

$$a \le b: \Leftrightarrow p_i(a) \le p_i(b) \quad \textit{for all } p_i \in IB \qquad (2)$$

The definition (2) denotes a *component-wise* or product order. By (2) the quasi-ordered set (qoset) is solely determined by P and IB. Therefore the qoset is written as (P, IB). The definition (2) induces the following graph theoretical setting.

Let P be the set of vertices of a graph G, then a directed edge ("arrow") from $a \in P$ points to b P if (2) is fulfilled. The resulting graph G(P, E), E the set of edges, is a directed acyclic graph. Note that a vertex may represent an equivalence class, according to eq 2.

One of the main purposes of ranking, namely the identification of priority elements can now be easily grasped: Let $v^+(x)$ be the number of incoming arrows of vertex x, and $v^-(x)$ that of outgoing arrows, then (large numerical values of evaluative properties meaning high contribution to the risk)

$PR \subseteq P$, PR: $= \{x \in P, v^-(x) = 0\}$,
the set of priority elements

$MAX \subseteq P$, MAX: $= \{x \in P, v^-(x) = 0, v^+(x) > 0\}$,
the set of (proper) maximal elements

$ISO \subseteq P$, ISO: $= \{x \in P, v^-(x) = v^+(x) = 0\}$,
the set of isolated elements

$MIN \subseteq P$, MIN: $= \{x \in P, v^+(x) = 0, v^-(x) > 0\}$,
the set of proper minimal elements (3)

Clearly the four sets PR, MAX, etc. depend on the sets P and IB, therefore the notation MAX(P, IB), for example, is useful.

The graph G(P, E) contains unnecessarily many edges. A—so called—transitive reduction[10] eliminates all edges which arise solely from the transitivity, see eq 1(3). Properly drawn, a reduced graph results, called a Hasse diagram, and it is denoted by H(P, IB).[11] G(P, E) is a "transitive hull" of H(P, IB). An EDV-code developed by Brüggemann, Halfon, and Bücherl is available from the first author. It performs all needed calculations and draws several types of graphs, especially the Hasse diagram.

Table 1. Chemicals of P′, Their Identifier, and Their Tuples $p(x)$

chemical	identifier	$T_{0.5}$ [days]	aqueous solubility [mg L^{-1}]	vapor pressure [mPa]	usage [tons* yr^{-1}]
alachlor	a0	15	240	−1.87	1537
atrazine	a4	60	33	−0.039	725
captan	b3	2.5	5.1	−0.011	557
carbaryl	b4	10	120	−0.16	590
mancozeb	h2	70	6	0	3465
metham-Na	i0	7	963 000	−0.000 002 7	5075
TCA	i4	21	1 200 000	0	889
methylbromide	i5	55	13 400	−243 000 000	3984
metolachlor	i7	90	530	−4.18	544
propanil	k6	1	200	−5.3	694
thiram	m1	15	30	−1.33	1180
ziram	n0	30	65	−0.0013	3151
zineb	n1	30	10	−0.01	2359

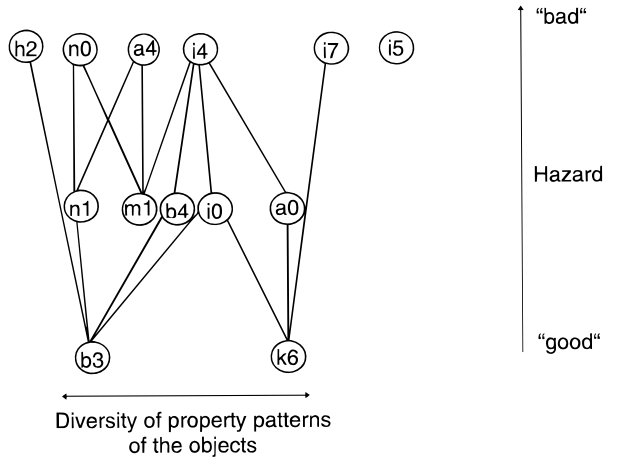

Figure 1. Hasse diagram of the qoset (P′, IB′), which actually is a poset, because there appears no nontrivial equivalence classes.

Example. Pesticides, mainly used in Italy, were already evaluated by the use of Hasse diagrams, and several conclusions have been drawn.[12] In this paper, not the full set of 50 pesticides but some subsets will be used, according to their suitability to demonstrate some facts.

As evaluative properties there were originally selected the

- persistence *T*, quantified by half-life in soils [d]
- aqueous solubility *W*, mg/L
- vapor pressure of the pure substances *V*, in mPa, and
- the yearly usage *U* (tons/year).

The vapor pressure is multiplied by −1 because—according to the protective aim—a low vapor pressure may lead to an accumulation in soils. The basic set P° is formed by 50 pesticides and the basic IB° is {*T*, *W*, *V*, *U*}. (A notational remark: By P,IB any object set and any information base are meant. Numerical indices differentiate them, if necessary.) As subset $P' \subset P°$ the set of 13 pesticides is selected. These pesticides have a yearly usage > 500 tons/year (see Table 1). The actual $IB' \subset IB°$ will be {*T*, *W*, *V*}.

According to P′, IB′, and (2) the Hasse diagram (Figure 1) results. It follows that six of 13 pesticides are priority elements (eq 3): PR(P′, IB′) = {h2, n0, a4, i4, i7, i5}. By

their combination of properties they are the worst chemicals; however, they mutually are not comparable. There is only one isolated element, i5; and there are three elements of MIN(P′, IB′), namely b3, m1, k6. So far the main goal of priority setting is reached. However, one can get much more information from this kind of graph.

•We note the isolatedness of i5, which implies a specific combination of properties namely a rather high aqueous solubility combined with a remarkably high vapor pressure.

•The pesticides, h2 and i7, are "almost" isolated, because both chemicals are comparable only with b3 and k6, respectively. Therefore it is useful to examine not only i5 but also h2 and i7 with respect to their data structure. In fact, for example, the pesticide h2 has a very low aqueous solubility combined with a long half-life.

•There are subsets of P′, of which each element can be compared with each other. These subsets are called chains. There are six chains which include three elements: C_1 = {b3, n1, n0}, C_2 = {b3, n1, a4}, etc. Such chains are of interest, because they include only objects, for which a *simultaneous* increasing *of all* $p_i \in$ IB is found. The chains clearly depend on P and IB; therefore, we write C_i(P′, IB′).

•Antichains are subsets of P′ of which no element is comparable to another. Often such antichains are also of interest, because they arise from the diversity of the properties: Let x,y be two objects which are incomparable (denoted as: x || y) and which therefore belong to an antichain. Then a high value of p_i(x) and a low value of p_j(x) may correspond to a low value of p_i(y) and a high value of p_j(y). For example, PR or {n1, b4, i0, a0} are antichains. Generally antichains are denoted as AC_i(P′, IB′). More specific and application-oriented examples may be found in the literature.[13,14]

The system of MAX, MIN, ISO, C_i, AC_i provides the structure of a qoset.

There arise six questions:

(1) What happens if any new property is added to the IB?

− stability analysis

(2) What is the importance of properties for the structure of the qoset and therefore for the results of the comparative evaluation?

− sensitivity analysis

(3) How does the ranking depend on the kind of data representations? The ordinal interpretation of data by (2) will differentiate between objects which have insignificantly different data.

− analysis of robustness

(4) Are there combinations of other and fewer properties which lead to the same qoset (to an isomorphic Hasse diagram)?

− dimension analysis

(5) Which variety of aggregations ares possible just to get a chain (total order), which encompasses all elements of a set P?

− aggregation analysis

(6) What can be said about the uncertainty of the rank of any element if a total order is constructed by aggregations?

− uncertainty analysis

In the following the first three questions will be discussed maintaining the graph theoretical visualization by Hasse diagrams. However a full treatment will be far beyond the scope of this paper. Interested readers will find details of (1) and (2) in refs 15−17. The questions (4)−(6) will be briefly mentioned in the final discussion.

STRUCTURAL ANALYSIS OF QOSETS

Stability Analysis. Goal. What can be expected, if a property will not be used in the product order, or if a property will be added to the IB. In other words, the stability of ranking results against decreasing or increasing the IB is to be estimated.

Idea. Find a characteristic quantity x(P, IB) which varies from 0 for a total order to 1 for a total antichain, for which is valid (IB_T: the fictitious set of all properties available):

$$IB_T \supset IB_1 \supset IB_2 \supset \{p_i\} \Rightarrow 1 \leftarrow x(P, IB_T) \geq x(P, IB_1) \geq x(P, IB_2) \geq x(P,\{p_i\}) \geq 0 \quad (4)$$

If x(P, IB) is near 0, then the structure of H(P, IB) may be rather stable against omitting a property but rather unstable against adding a property. If x(P, IB) is near 1, then the structure of H(P, IB) may be rather stable against adding but rather unstable against deleting any property.

Realization. Clearly there are many possibilities to realize this idea. We begin with four global quantities which characterize (P, IB). Within a qoset there are four possibilities for any two objects a,b ∈ P: (1) a ≤ b or (2) b ≤ a, comparability; (3) a || b, incomparability; (4) a ∼ b, equivalence. Therefore for the directed (graph theoretical) simplex with $N^*(N-1)$ (=:$S(N)$) edges a balance equation can be found, with N being the number of objects. This equation relates $S(N)$ with the number of comparabilities V(P, IB) and that of incomparabilities U'(P, IB). Some care is needed regarding the equivalence classes. The result is eq 5 (for more details: see ref 17):

$$S(N) = 2^*U'(P, IB) + 2^*V(P, IB) - K(P, IB) \quad (5)$$

with K(P, IB): $= \sum N_i^*(N_i - 1)$ and N_i the number of elements in the ith equivalence class. A realization of x(P,-IB) can be found from (5) by setting

$$\Xi := 2^*U'(P,IB)/S(N)$$

As can be shown from eq 5 the quantity Ξ, ranges from 0 to 1. It measures the extent of "chainicity" or of "antichainicity" and relates this feature by (4) to the extent of the information base.

Example. The qoset, whose visualization H(P′, IB′) is shown in Figure 1, has the following global quantities: V(P′, IB) = 19; U'(P′, IB′) = 59; K(P′, IB′) = 0; $S(N)$ = 156; Ξ(P′, IB′) = 0.756. We conclude, that the ranking may be rather stable against an additional property, but unstable against omission of a property already included in IB′, because H(P′, IB′) has more "antichain" than "chain"-character. Hence the information base to rank the 13 pesticides seems to be rather complete.

To demonstrate the stability/instability an additional property is needed. The only one property available is the usage, U. Applying the extended information base, the comparative evaluation of the 13 pesticides leads to the following results (see Figure 2):

$$PR(P', IB' \cup \{U\}) = PR(P', IB') \cup \{i0, a0\}$$

$$ISO(P', IB' \cup \{U\}) = ISO(P', IB') \cup \{i7\}$$

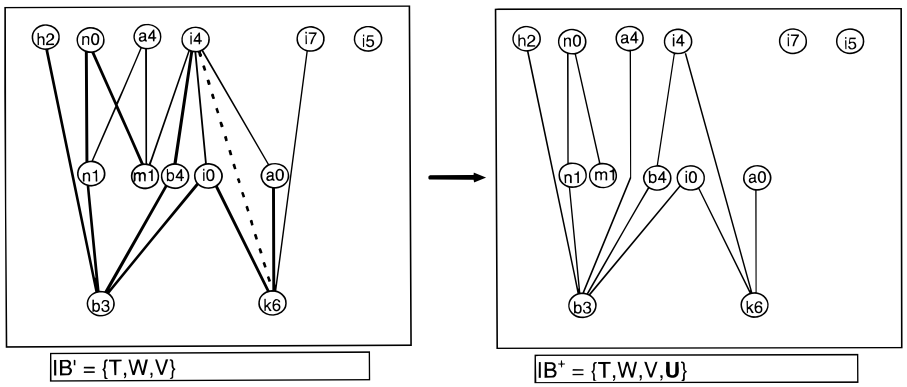

Figure 2. The effect of extending the information about pesticides by adding the yearly usage to the information base IB′.

$$\mathrm{MIN}(P', IB') = \mathrm{MIN}(P', IB'')$$

Two of six three-element chains survive: $C_1(P',IB' \cup \{U\}) = \{b3, n1, n0\}$ and $C_2(P',IB' \cup \{U\}) = \{b3, b4, i4\}$. All in all, it can be verified that the qoset (P′, IB′) is rather stable against the one new property. By help of sensitivity analysis the amount of alterations can be further quantified. The effect of the omission of any one particular property is summarized in Table 2. The corresponding three Hasse diagrams (see Figure 4) look very chain-like in the first two cases. In the third case a balanced mixture of chains and antichains arises. Obviously the neglect of the property "vapor pressure" induces few modifications (third case) but neglect of any of the other two properties leads to a rather dramatical changing of the structure of the qoset (P′, IB′). The index Ξ (P′, IB′) *warns of such effects, but does not quantify* the structural changes. This is the task of the sensitivity analysis, where subsets of IB are examined.

Remarks. Whereas the effect of omitting a subset of properties of a given IB can also be analyzed by sensitivity analysis, the effect of an a priori unknown evaluative property can only be estimated by quantifying the neighborhood to a total antichain. Total antichains from P may even arise if two properties are exactly anticorrelated, but in general this specific structure will only be achieved, if very large IBs are considered. This may correspond to the more or less philosophical statement, that each object is an individual and cannot be compared to others, if *all* its properties are considered.

Sensitivity Analysis. Goal. To assess the importance of each attribute for the structure of a qoset.

Idea. By ρ(IB), the power set of IB, a family of qosets arises: $(P_1\ IB_S)_1\ IB_S \subseteq \rho(IB)\backslash\phi$. With ϕ the empty set is denoted. Let **P** be this family of posers, then a distance function D: $\mathbf{P} \times \mathbf{P} \rightarrow$ IR can be introduced. With the aid of D the special distances of qosets (P, IB) to (P, IB(i)) can be measured (IB(i) $\in \rho$(IB) and IB(i): $=$ IB$\backslash\{p_i\}$). Large values of D indicate that the omitted property p_i has a large influence, whereas low values would assign p_i a minor influence on the structure of the qoset and therefore on the result of a comparative evaluation.

Realization. There are again many possibilities to find an appropriate distance function (for an overview: see Monjardet[18]). However for ranking purposes it is useful to find a distance function as follows

Table 2. Effect of Omitting Properties of IB′ = {*T*, *W*, V}[a]

	{*W*, *V*}	{*T*, *V*}	{*T*, *W*}
U′	35	27	39
Ξ	0.45	0.32	0.5

[a] $U'(P', IB') = 59$.

$$D:\ \{(P_S, IB_{S1})\} \times \{(P_S, IB_{S2})\} \rightarrow IR, \quad \text{with } P_S \subseteq P \text{ and } IB_{S1}, IB_{S2} \subseteq \rho(IB) \quad (6)$$

Here a remark is necessary: The requirement "the distance between two objects A,B equals zero implies A = B" is too severe for the purposes here. We relax this demand to "..implies A equivalent to B" and maintain for the sake of simplicity the term "distance".

Thus the distance can also scan the sensitivity of any properties with respect to the location of the vertices $x \in P_S$. The sensitivity of a property p_i may be changed significantly if the whole set, or—for example—only PR is considered, i.e., if $P_S = P'$ or $P_S =$ PR (see example).

To achieve the desired distance function, consider the principal order ideal $o(x)$, i.e., the order ideal generated by one element, say x of P as

$$o(x) = \{y \in P, y \le x\}$$

In Figure 3 two examples of order ideals are shown. To discuss the different IBs, we extend the notation to $o(x; IB_S)$, $IB_S \subseteq IB$.

By $W(x, IB_{S1}, IB_{S2})$: $=$ card $(o(x, IB_{S1}) \Delta o(x, IB_{S2}))$, which is a distance between two order ideals, and because of the dependence on x, the relative importance of the different property-sets on the ranking of x can be found. The symbol Δ denotes the symmetric set difference, and its cardinality is called Hamming distance.[19]

For $x \in P_S \subseteq P$:

$$W(P_S, IB_{S1}, IB_{S2}) = \sum_{x \in P_S} W(x, IB_{S1}, IB_{S2})$$

is a generalization. The general properties of $W(P_S, IB_{S1}, IB_{S2})$ will be discussed in a forthcoming paper.[20]

If $IB_{S1} = IB_{S2} \cup \{p_i\}$, then the influence of this property, p_i, on the downward comparabilities of $x \in P_S$ is quantified by $W(P_S, IB_{S1}, IB_{S2})$. It may be worthwhile to note that the mapping (P, IB) $\rightarrow$ (P, IB_S), $IB_S \subset IB$ is order preserving, (meaning that any $x \le y$ in (P, IB) implies $x \le y$ in (P, IB_S)).

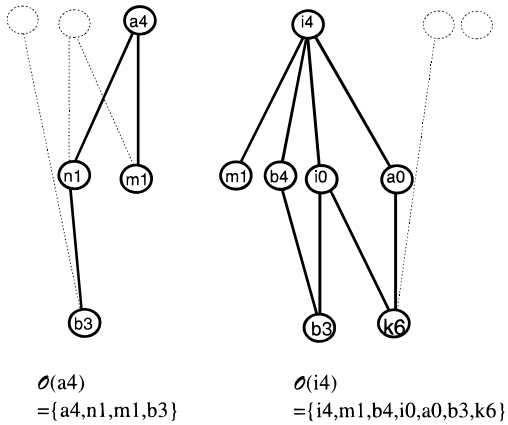

Figure 3. Examples of principal order ideals, each generated by exactly one element of P′. To facilitate the identification some other objects and edges are indicated.

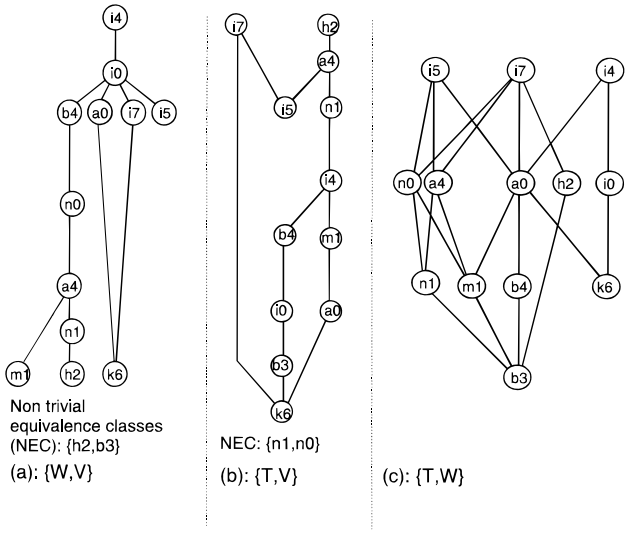

Figure 4. The visualization of the qosets (P′, IB(X)), $X = T$ (a), W (b), V (c). The different changes with respect to the diagram in Figure 1 should be recognized.

Table 3. W(P′, IB′, IB(X)) as a Realization of a Distance Function

	IB(T)	IB(W)	IB(V)
W	25	35	20

Example. The set P′ of 13 pesticides and IB′ = {T, W, V} are selected. First of all it is of interest to see the influence of each single property on the structure of the qoset. Therefore as P_S the whole set P′ is selected. As subsets IB_S are selected.

$$IB(T) = \{W, V\}; \quad IB(W) = \{T, V\}; \quad IB(V) = \{T, W\}$$

In Figure 4 the three resulting Hasse diagrams are shown. It is evident that H(P′, IB(V)) looks most similar to that of (P′, IB′). Whereas it is more difficult, to decide which of the two qosets (P′, IB(T)) or (P′, IB(W)) is more dissimilar to the original qoset. The calculated distances W(P′, IB′, IB(X)) $X = T, W, V$ are shown in Table 3. The neglect of aqueous solubility has the most influence, that of the vapor pressure the least influence. Obviously the vapor pressure does not differentiate enough among the chemicals, therefore the neglect will not change the qoset too much.

How will the priority elements PR(P′, IB′) be affected by the three properties? By the specific construction of the distance measure, W(PR(P′, IB′), IB′, IB(X)) $X = T, W, V$, this question can be easily answered (Table 4). The results show that with respect to the priority elements the importance of the properties has changed. Now, the persistence time is of only little importance, whereas the vapor pressure becomes relatively more important.

Table 4. W(PR(P′, IB′), IB′, IB′(X)) as a Realization of a Distance Function, Now Restricted to the Priority Elements Found in (P′, IB′)

	IB(T)	IB(W)	IB(V)
W	9	23	16

Analysis of Robustness. Goal. The comparative evaluation performed by application of eq 1 interprets ordinally even insignificant differences in numerical values of the data. This often results in very complicated diagrams, and often misleading interpretations are possible. An approach is to classify each property separately or to perform a cluster analysis. However the main question is which classification or which cluster-partitioning is appropriate to start an order analysis. Therefore the goal is to find additional tools to select the appropriate data representation.

Idea. Use the distance function, mentioned above, but for qosets with different data representations. Each data representation with respect to all evaluative properties is denoted as A, which contains information about the numerical manipulations of each single property.

Realization. The extended notation (PS, IB′, A), $P_S \subseteq$ P, allows the following setting:

$$D(A,A'): \{(P_S, IB, A)\} \times \{(P_S, IB, A')\} \rightarrow IR \quad (7)$$

To relate (7) to the distance measure already introduced, the IB will be formally extended to (IB, IB), where for p_{n+1}, p_{n+2}, to p_{2n} the classified values or representative values for clusters are taken. The modified data p_{n+1}, p_{n+2}, to p_{2n} correspond to the data representation A'. Then the distance, D: (P_S, $\{p_1,p_2,...,p_n\}$,$\{p_{n+1},p_{n+2},..,p_{2n}\}$) → IR, can be calculated as done for the sensitivity analysis. As an abbreviation we introduce $\Gamma := D(A,A') = W[P_S,\{p_1,p_2,...,p_n\},\{p_{n+1},p_{n+2},..,p_{2n}\}]$. Γ is a dissimilarity measure for qosets arising from different data representations.

Example. There are many possibilities to perform classifications. *Here* an equidistant classification, A^{ec}, for each of the three attributes {T,W,V} is used to exemplify the idea and its realization. As P_S the set P′ is selected. The equidistant classification into—for example—k classes means the following: The interval (p_i(min), p_i(max)) will be divided into k subsequent equidistant intervals I_1,I_k and instead of the actual value of p_i the corresponding interval number will characterize the object:

$$\text{Let } \delta_k(i) = (p_i(\max) - p_i(\min))/k \quad \text{then } p_i(a) \rightarrow$$
$$j_i(a) \quad \text{if} \quad p_i(a) \in I_j^{(k,i)}: = [\delta_k(i)*j,\ \delta_k(i)*(j+1))$$

The quantity Γ tends to zero, as finer intervals $I_j^{(k,i)}$ are chosen. Beyond this it can be observed that the mappings (P, IB, A^o) → (P, IB, A^{ec}) are order preserving. Clearly a global minimum with a data representation A' unequal to the original one A cannot be expected. However local minima, very flat parts, and steep gradients of Γ versus increasing k can be found as Figure 5 shows (the same k for all three properties). For example the local minimum at class

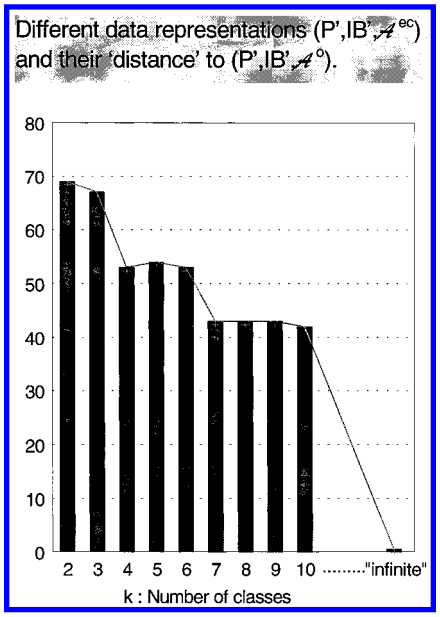

Figure 5. $D(\mathcal{A}^{o}, \mathcal{A}^{ec})$ is shown in dependence of *k*. The same *k* for each of the three properties. The fine line helps to identify the only one local minimum and a series of constant values.

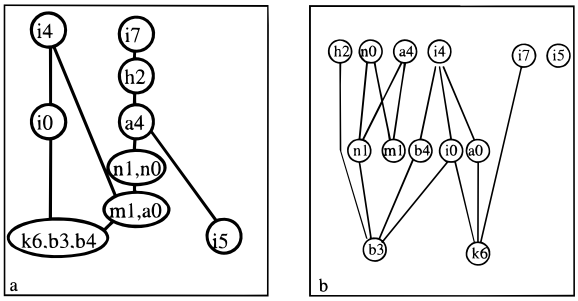

Figure 6. All three properties of IB′ divided into seven equidistant classes: (a) one example of data representations $\mathcal{A}^{ec}$ and (b) H(P′, IB′) just for comparison.

number 4 or the class number 7 beginning a flat part of the graph shown in Figure 5 may be selected as candidates. For example, the visualization of the qoset in the latter case is shown in Figure 6.

Remark. Generally a presentation as shown in Figure 5 is not possible, because the different possibilities to classify data, to perform clusterings, etc. cannot be ordered linearly. The distance function Γ helps to find a way on a local scale (for example, in a neighborhood of a actual *j*-value) through the jungle of different data representations. What is needed would be an additional criterion to find an optimized qoset on a global scale.

DISCUSSION

Not all facets of the theory of partially ordered sets could be shown. Totally missing is the link to the powerful instruments of statistics. Here still much work is needed. The dimension analysis of posets (see for example ref 21) may help to recognize redundancies of the IB, which may initialize statistical investigations. For example, if (P, IB) (card IB = $n > 2$) had dimension 2 then a two-dimensional representation of the objects must be possible, and a mapping may be found, relating p_j ($j = 1,...,n$) to new properties η_i, ($i = 1,2$) such that (P, IB) is isomorphic to (P,$\{\eta_1,\eta_2\}$).

Many examples show the fruitfulness for ecosystemic considerations of even such simple mathematical structures as shown here. There is also a close connection to lattice theory, especially of the Formal Concept analysis (see for example refs 22−25), which can be extended to a type of artificial intelligence.

Still more important is the embedding of the concept of comparative evaluation by partial ordering into probabilistic concepts. The tools for how to do this are already known. The basic idea is to assign to (P, IB) the set of all total orders which maintain the comparabilities of the original qoset/poset. From this set characteristic quantities can be extracted, and expectation values of an average rank of an element of P are derived (see for example ref 26). Furthermore it is possible to estimate the uncertainties of the ranks. Such uncertainties arise, if a partial order is mapped onto a total order by aggregation. For example, elements which have a high degree of incomparability, as for example for the pesticides h2 and i7 in (P′, IB′)), have a large span of their rank over all possible total orders.[27] Therefore each aggregation procedure, even if well defined, should be accompanied by an analysis of partial or quasi orderings.

The extension of the application of partially ordered sets to different sections of environmental chemistry is still ongoing. It may be worthwhile to mention that applications in the field of QSAR are in the beginning.[28−30]

Partial orders play not only an increasing role in chemistry as D. J. Klein shows[31,32] but also in an important field of ecology, namely food web theory. Food webs in turn are important when an ecosystemic risk assessment on a very general basis is desired.[33] Not the product order but the interval order is then a leading concept, and if food webs are really "roadmaps through Darwin's, famous entangled banks",[34] then order concepts are one of the main vehicles to explore them.

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