

# Dominance and separability in posets, their application to isoelectronic species with equal total nuclear charge

Guillermo Restrepo · Rainer Brüggemann

Received: 27 March 2007 / Accepted: 15 October 2007 / Published online: 8 December 2007  
© Springer Science+Business Media, LLC 2007

**Abstract** We developed the dominance and separability degrees as two new mathematical tools measuring the amount of comparabilities and incomparabilities among pairs of disjoint subposets in a parent poset and we have related them through a theorem. Their mathematical properties when these measures are constrained to be higher than 0.5 have been studied. We have shown that variations of dominance and separability degrees from values in the real interval  $(0.5, 1]$  permit to “tune” the level of detail on the comparabilities and incomparabilities among the subsets studied. The lack of transitivity of dominance and separability degrees is established, along with the special requirement, needed on the poset, to have a transitivity of these measures. As a chemical application, the Hasse diagram of Born-Oppenheimer molecular total energies of the complete set of isoelectronic species with total nuclear charge 10 in their minimum energy configurations has been studied. We partition this set into 10 subsets, each one containing all the species with the same number of nuclei. By the calculation of the dominance and separability degrees a relation between the number of atoms in any ensemble and the Born-Oppenheimer energies is established.

**Keywords** Partially ordered sets · Posets · Ranking · Born-Oppenheimer energies

---

G. Restrepo (✉)  
Laboratorio de Química Teórica, Universidad de Pamplona, Pamplona, Colombia  
e-mail: grestrepo@unipamplona.edu.co

G. Restrepo  
Environmental Chemistry and Ecotoxicology, University of Bayreuth, Bayreuth, Germany

R. Brüggemann  
Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany

*Present Address:*

G. Restrepo  
Lehrstuhl für Umweltchemie & Ökotoxikologie, Universität Bayreuth, Bayreuth, 95440, Deutschland

## 1 Introduction

Partially ordered sets (posets) are mathematical structures based on a comparison among the elements of a set [1]. If these elements are defined by their properties, then a poset is the result of the simultaneous comparison of the elements through their properties. Comparisons are usual in human activities, examples of their presence are these kinds of questions: which is the best kind of economic system?, which is the best university?, which is the best quantum-chemical level of calculation?, which is the most hazardous substance? In order to reply to these questions it is always necessary to make comparisons, and a poset is the mathematical structure behind them.

There are several posetic studies in different fields of knowledge [1,2]; in economy, for instance, Annoni recently ranked and classified a set of European countries according to their public level of satisfaction regarding different public services [3]; in ecology, Solomon has pointed out the posetic character of the abundance vectors used to define a community in diversity studies [4]; in thermodynamics and quantum mechanics it has been shown the relation of the Young diagrams lattice (a poset) with the mixing character [5–7] and the generation of wave functions satisfying the Pauli exclusion principle [8]. Particularly in chemistry, instances of posetic studies started at the end of 1960s with Ruch and his investigations into the algebraic description of chirality [9,10]; afterwards Randić and some others made important researches on chemical structure and its posetic description [11–15]. Another relevant and nowadays quite explored aspect of posets in chemistry was initiated by Halfon and Reggiani in 1986 when they ranked substances in environmental hazard studies [16]; this line of research has been deeply studied by Brüggemann and coworkers [1,17–29], who regularly organise workshops about posets in chemistry and environmental sciences. Some other instances of these mathematical structures in chemistry are found in Refs. [1,28–36]. A more general statement on posets has been set up by Klein and Babić [35,36], who have pointed out that posets may be deeply related to experimental sciences through the measuring process. According to these authors, ambiguities resulting from measurements might be explained as the result of measuring elements, which in reality must be considered as incomparable. Hence, the measuring method may force the incomparabilities to be comparable and, because of the different possibilities to do this [37,38], the outcomes may be different, therefore “ambiguous”, in a systematically controlled way.

Once a poset is detected or constructed on a given set, its analysis permits to draw conclusions on the order relations among the elements considered, for instance maximal and minimal elements or order intervals, ideals or filters [39]. The study of these posetic features and their properties are an important and active research field of mathematics, mainly carried out in combinatorics. However, to our knowledge, there is little information on the study of posetic properties of subsets of elements belonging to a poset. That is to ask, if the original set is partitioned into different subsets, what is the behaviour of the order relations among these subsets? In a chemical framework this question can be exemplified as: given a poset of organic molecules, which are the order relations between alkanes–alkenes, alkanes–alkynes, alkynes–amines and so on? In this paper we deal with that question and we develop two measures, one related to the comparability and another one with the incomparability between a pair of subsets;

the first measure is called the dominance degree and the second one the separability degree. We also describe their mathematical properties and their relation through a novel theorem. Finally, these measurements are applied to different subsets of a poset of isoelectronic chemical species with equal total nuclear charge.

## 2 Methodology

For the sake of clarity we introduce some terms useful for the understanding of the paper:

**Definition 1** An ordered pair  $(P, R)$  is called a *structure* if  $R$  is a relation on the non-empty set  $P$  which is called a ground set and is here considered finite.

**Definition 2** A binary relation  $\leq$  on  $P$  is called a *partial order* if:

1.  $x \in P \Rightarrow x \leq x$ ,
2.  $x, y \in P, x \leq y$  and  $y \leq x \Rightarrow x = y$ ,
3.  $x, y, z \in P, x \leq y$  and  $y \leq z \Rightarrow x \leq z$ .

Then  $\leq$  is respectively reflexive, antisymmetric and transitive on  $P$ . A ground set equipped with a partial order is called a *poset* (partially ordered set) and it is denoted as  $(P, \leq)$ .

**Definition 3** Let  $P'$  be a subset of  $P$ , with the inherited order relation  $\leq$ , then  $(P', \leq)$  is a subposet of  $(P, \leq)$ .

In some cases the fact of having  $x \leq y$  and  $y \leq x$  does not necessarily imply  $x = y$ . In those situations it is said that  $x$  and  $y$  are related by an equivalence relation different than equality, for instance a similarity relation [40] in which case  $\leq$  is called a quasi order [19]. This may occur when the elements of  $P$  are described by means of their features. In the case with a quasi-order one may define an equivalence relation  $\approx$  such that the equivalence class of  $x \in P$  is  $\{y : x \leq y \text{ and } y \leq x\}$ . Hence, if one wants to order the elements of  $P$  according to  $\leq$ , it is possible to select a representative element of each equivalence class to perform the ordering, instead of considering all the elements in  $P$ , including equivalent ones. In that case the relation  $\leq$  is not applied to the complete set  $P$  but to a set  $P''$  of representative elements of each equivalence class. In order to avoid cumbersome notation, we keep calling  $P$  the reduced set  $P''$  of representatives.

**Definition 4** Two elements  $x, y \in P$  are said to be *comparable* if either  $x \leq y$  or  $y \leq x$ . We say that  $x$  *surpasses*  $y$  if  $y \leq x$ .

**Definition 5** Given two elements  $x, y \in P$ , we say that  $y$  is *covered* by  $x$ , denoted  $y \leq: x$ , if  $y \leq x$  and there is no  $z \in P$  for which  $y < z$  and  $z < x$ . If  $y \leq: x$ , it is said that  $x$  *covers*  $y$ .

The existence of  $(P, \leq)$  does not guarantee the comparability between every pair  $x, y \in P$ . For those “incomparable” elements a new relation is defined.

**Definition 6** For all  $x, y \in P$ ,  $x$  and  $y$  are *incomparable* ( $x||y$ ) iff not  $x \leq y$  and not  $y \leq x$ . The *incomparability* relation  $||$  is a binary relation on  $P$  fulfilling these properties:

1.  $x \in P \Rightarrow \text{not } x||x$ ,
2.  $x, y \in P, x||y \Rightarrow y||x$ .

Then  $||$  is an irreflexive and symmetric relation on  $P$ .

**Definition 7** Let  $G_{\leq} = (P, E_{\leq})$  the *comparability graph* of  $(P, \leq)$ , where  $E_{\leq}$  is the set of edges containing the comparable pairs in  $P$ .

**Definition 8** Let  $G_{\leq} = (P, E_{\leq})$  the *cover graph* of  $(P, \leq)$ , where  $E_{\leq}$  is the set of edges containing the cover pairs in  $P$ .

$G_{\leq}$ , as well as  $G_{\leq}$ , is an undirected graph which offers more information about comparabilities and incomparabilities if it is oriented taking advantage of the antisymmetry of  $\leq$  [2].

**Definition 9** Let  $H = (P, d(E_{\leq}))$  a directed graph of  $(P, \leq)$  where  $d(E_{\leq})$  is the set of directed edges containing the cover pairs in  $P$ .  $H$  is called the *Hasse diagram* of  $(P, \leq)$  if it is drawn in the Euclidean plane whose horizontal/vertical coordinate system requires that the vertical coordinate of  $x \in P$  be larger than the one of  $y \in P$  if  $y \leq x$ .

**Definition 10** Let  $G_{||} = (P, E_{||})$  the *incomparability graph* of  $(P, \leq)$ , where  $E_{||}$  is the set of edges containing the incomparable pairs in  $P$ .

## 2.1 Order relations among subsets of a poset

There are two ways for studying the order relations among subsets of a poset  $(P, \leq)$ . The first one clusters the elements of  $P$  and defines pseudo-objects as centres of the clusters and finally analyses the resulting partial order on the set of pseudo-objects [20]. The second possibility considers all the order relations between members of different subsets of  $P$ , which can arise from external knowledge. For example, chemicals may be ordered due to a set of properties. There may still be information, which is not used for ordering the chemicals but which can be used to define subsets within the partially ordered set. This methodology and its properties are studied in this paper by defining two new structural parameters of  $(P, \leq)$ ; one dealing with the  $\leq$ -relation between subsets, called dominance<sup>1</sup> degree, and another one studying the  $||$ -relation, called separability degree. Since these two measures depend on the number of comparabilities and incomparabilities among the elements of any two subsets of a Hasse diagram, we introduce an indicator function useful for counting them.

<sup>1</sup> The concept of dominance developed in this paper is not directly related to the one of dominating set, which is as follows [41]: A *dominating set* is a set of vertices  $D \subseteq V$  in a graph  $G = (V, E)$  having the property that every vertex  $v \in V - D$  is adjacent to at least one vertex in  $D$ .

**Definition 11** Let  $(P, \leq)$  be a poset with  $P_i$  and  $P_j \subset P$  such that  $P_i \cap P_j = \emptyset$ . Then for all  $x \in P_i, y \in P_j$  it is defined the *indicator function*  $L_{xy}^{(i,j)}$  as follows:

$$L_{xy}^{(i,j)} = \begin{cases} 1 & \text{if } y \leq x \\ -1 & \text{if } x \leq y \\ 0 & \text{if } x \parallel y \end{cases} \tag{1}$$

Whenever it holds a comparability between  $x$  and  $y$ ,  $L_{xy}^{(i,j)}$  assigns a value of 1 or  $-1$ , being 1 when  $x$  surpasses  $y$  and  $-1$  when  $y$  surpasses  $x$ ;  $L_{xy}^{(i,j)}$  yields a value of zero when the pair is incomparable (recall that equivalences are excluded). This kind of indicator function is used in observational studies [42] and it is further described by Rosenbaum [42,43].

In order to have an account of the number of comparabilities ( $y \leq x$  and  $x \leq y$ ) and incomparabilities ( $x \parallel y$ ) in  $P$ , the statistics  $T_{j \leq i}, T_{i \leq j}$  and  $T_{i \parallel j}$  are created.

**Definition 12** Let  $P_i$  and  $P_j$  be two disjoint subsets with  $x \in P_i, y \in P_j$  and respective cardinalities  $n_i$  and  $n_j$ . The statistics  $T_{j \leq i}, T_{i \leq j}$  and  $T_{i \parallel j}$  among all possible  $n_i \cdot n_j$  relations are defined as:

$$\begin{aligned} T_{j \leq i} & \text{ is a count of all } L_{xy}^{(i,j)} = 1, \\ T_{i \leq j} & \text{ is a count of all } L_{xy}^{(i,j)} = -1, \\ T_{i \parallel j} & \text{ is a count of all } L_{xy}^{(i,j)} = 0. \end{aligned} \tag{2}$$

In the following we introduce the dominance and separability degrees.

**Definition 13** Let  $(P, \leq)$  be a poset with  $P_i, P_j \subset P$  such that  $P_i \cap P_j = \emptyset$  and  $n_i = |P_i|, n_j = |P_j|$ . Then for all  $x \in P_i$  and  $y \in P_j$ , the *dominance degree* of  $P_i$  over  $P_j$  is given by

$$Dom(P_i, P_j) = \frac{T_{j \leq i}}{n_i \cdot n_j} \tag{3}$$

Hence,  $Dom(P_i, P_j)$  counts the number of ordered pairs where an element of  $P_i$  surpasses an element of  $P_j$  and divides it by all the possible relations between  $P_i$  and  $P_j$ . Therefore,  $Dom$  yields a real value ranging from 0 to 1;  $Dom(P_i, P_j) = 1$  means that all the elements in  $P_i$  surpass all those in  $P_j$ . In contrast, if  $Dom(P_i, P_j) = 0$ , it means that no element of  $P_i$  surpasses an element of  $P_j$ . Note that, because of the anti-symmetry of  $\leq$  (Definition 2),  $Dom(P_i, P_j)$  is not necessarily equal to  $Dom(P_j, P_i)$  and the equality only occurs when the number of pairs  $x \leq y$  is equal to the number of pairs  $y \leq x$  (see Corollary 1).

The relations defined on  $P$  are of two types: comparabilities ( $\leq$ ) and incomparabilities ( $\parallel$ ). Since  $Dom(P_i, P_j)$  represents the fraction of relations of  $P_i$  over  $P_j$  such that  $y \leq x$  with  $x \in P_i$  and  $y \in P_j$ , it is possible that the rest of the relations correspond to either comparabilities where the elements of  $P_j$  surpass those of  $P_i$ , or

incomparabilities among them. Hence, given a value of  $Dom(P_i, P_j)$  it is natural to ask for  $Dom(P_j, P_i)$  and also for the proportion of incomparabilities. These incomparabilities may be gathered in a mathematical expression similar to and, as we show later in Theorem 1, related to dominance degree.

**Definition 14** Given a poset  $(P, \leq)$  with  $P_i, P_j \subset P$  such that  $P_i \cap P_j = \emptyset$  and  $n_i = |P_i|, n_j = |P_j|$ , then for all  $x \in P_i, y \in P_j$ , the *separability degree* between  $P_i$  and  $P_j$  is given by

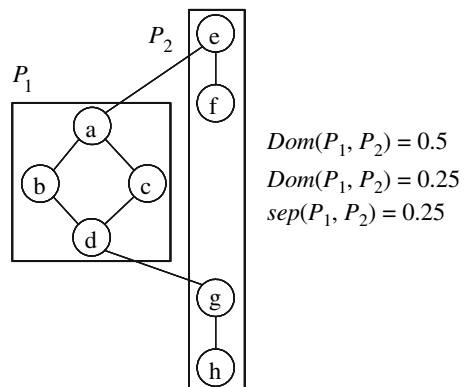
$$Sep(P_i, P_j) = \frac{T_{i||j}}{n_i \cdot n_j} \quad (4)$$

$Sep(P_i, P_j)$  is the result of the division of the number of incomparabilities between the elements of  $P_i$  and  $P_j$  and the number of order relations between  $P_i$  and  $P_j$ . Note that  $Sep(P_i, P_j) = Sep(P_j, P_i)$  because of the symmetry of  $||$  (Definition 6). Separability degree takes values in the real interval  $[0, 1]$ ;  $Sep(P_i, P_j) = 1$  means that all the possible relations between  $P_i$  and  $P_j$  are incomparabilities; in contrast, a value of  $Sep(P_i, P_j) = 0$  means that there are no incomparabilities between  $P_i$  and  $P_j$ , thereby all their relations are comparabilities and they are counted in  $Dom(P_i, P_j)$  and  $Dom(P_j, P_i)$ . Hence, there is a mathematical relation between  $Dom(P_i, P_j), Dom(P_j, P_i)$  and  $Sep(P_i, P_j)$ , which is set up in Theorem 1. Before introducing this theorem and its consequences, we show an example of calculation of dominance and separability degrees.

*Example 1* Let  $P = \{a, b, c, d, e, f, g, h\}$ ,  $P_1 = \{a, b, c, d\}$ ,  $P_2 = \{e, f, g, h\}$  and the Hasse diagram depicted in Fig. 1. In this case  $Dom(P_1, P_2) = 8/16 = 0.5$ ,  $Dom(P_2, P_1) = 4/16 = 0.25$  and  $Sep(P_1, P_2) = 4/16 = 0.25$ .

Note that the only requirement for calculating dominance and separability degrees is that  $P_i$  and  $P_j$  be disjoint subsets. This implies that their internal relations,  $\leq$  and  $||$ , are not necessary for building up  $P_i$  or  $P_j$ . In fact, they might be antichains, chains or mixtures of them and this fact does not address the membership to  $P_i$  or  $P_j$ .

**Fig. 1** A Hasse diagram on the set  $P = \{a, b, c, d, e, f, g, h\}$ ; two “boxed” subsets  $P_1 = \{a, b, c, d\}$  and  $P_2 = \{e, f, g, h\}$  with  $n_1 = n_2 = 4$ ; and their respective dominance and separability degrees



**Theorem 1** Let  $(P, \leq)$  be a poset with  $P_i, P_j \subset P$  such that  $P_i \cap P_j = \emptyset$ . The dominance (*Dom*) (Definition 13) and separability (*Sep*) (Definition 14) degrees for  $P_i$  and  $P_j$  satisfy  $Dom(P_i, P_j) + Dom(P_j, P_i) + Sep(P_i, P_j) = 1$ .

*Proof*  $Dom(P_i, P_j)$ ,  $Dom(P_j, P_i)$  and  $Sep(P_i, P_j)$  are defined on  $P_i, P_j \subset P$ , where  $n_i = |P_i|$  and  $n_j = |P_j|$ . There are two relations defined on  $P$ , namely  $\leq$  (Definition 2) and  $\parallel$  (Definition 6), which are in turn defined on the subposets  $(P_i, \leq)$  and  $(P_j, \leq)$ . The relation  $\leq$  can be split into the relations  $\leq_{ji}$  and  $\leq_{ij}$ , where  $\leq_{ji} = \{(x, y) : x \in P_i, y \in P_j \text{ and } y \leq x\}$  and  $\leq_{ij} = \{(x, y) : x \in P_i, y \in P_j \text{ and } x \leq y\}$ . Then, the set  $\{\leq_{ji}, \leq_{ij}\}$  is a partition of  $\leq$  because  $\leq = \leq_{ji} \cup \leq_{ij}$  and  $\leq_{ji} \cap \leq_{ij} = \emptyset$ . From this, and from Definition 6, follows that  $\leq \cap \parallel = \emptyset$  and  $R = \leq \cup \parallel$ , where  $R = \{(x, y) : x \in P_i, y \in P_j \text{ and either } y \leq x \text{ or } x \leq y \text{ or } x \parallel y\}$ , which is the set of ordered pairs  $(x, y) \in P_i \times P_j$  fulfilling the relations  $\leq$  and  $\parallel$ . Then,  $\{\leq_{ji}, \leq_{ij}, \parallel\}$  is a partition of  $R$  because  $\leq_{ji} \cap \leq_{ij} \cap \parallel = \emptyset$  and  $R = \leq_{ji} \cup \leq_{ij} \cup \parallel$ . Since  $|R| = n_i \cdot n_j$ , then  $|\leq_{ji}| + |\leq_{ij}| + |\parallel| = n_i \cdot n_j$ , and, according to Definition 11, this is equivalent to  $T_{j \leq i} + T_{i \leq j} + T_{i \parallel j} = n_i \cdot n_j$ . Thus, from Definitions 13 and 14 it follows that  $Dom(P_i, P_j) + Dom(P_j, P_i) + Sep(P_i, P_j) = 1$   $\square$

The dominance degree,  $Dom(P_i, P_j)$ , is a measurement of the extent of comparability between any two disjoint subposets of  $P$ . In observational studies [42–44], whose goal is to measure the effect of a cause, for instance the effect of a medical treatment on patients, a set  $P$  of observations (patients) is divided into two subsets  $P_i$  (control) and  $P_j$  (treatment). When the observations are described by more than one outcome, then  $P$  may become a poset and the coherence of the cause-effect hypothesis is measured by the degree of dominance of one of the two considered subsets in the poset. This measurement is carried out by a statistic operating on the set of relations between the two compared subsets and it considers simultaneously comparabilities and incomparabilities. The statistic used in these studies [44] is:

$$\hat{\zeta}_C = \frac{\sum_{l=1}^{n_1} \sum_{m=1}^{n_2} L_{lm}^{(1,2)}}{n_1 \cdot n_2}, \text{ with } L_{lm}^{(1,2)} = \begin{cases} 1 & \text{if } y_m \leq x_l \\ -1 & \text{if } x_l \leq y_m \\ 0 & \text{if } x_l \parallel y_m \end{cases} \begin{cases} l \in I_1, m \in I_2 \\ I_j \equiv \text{index set for } P_j \end{cases} \tag{5}$$

Since  $\hat{\zeta}_C$  operates over all possible values of  $L_{lm}^{(1,2)}$ , it does not distinguish between  $L_{lm}^{(1,2)} = 1, -1$  or  $0$ , thereby it does not differentiate between  $Dom(P_i, P_j) = Dom(P_j, P_i)$ ,  $Sep(P_i, P_j) = 1$ ; and  $Dom(P_i, P_j) = Dom(P_j, P_i)$ ,  $Sep(P_i, P_j) = 0$ ; yielding a value of zero for both cases. It can be also noted that  $\hat{\zeta}_C = Dom(P_i, P_j) - Dom(P_j, P_i)$ . Then, the advantage of studying individually  $Dom(P_i, P_j)$ ,  $Dom(P_j, P_i)$  and  $Sep(P_i, P_j)$  makes it possible to go into the details of the comparability and incomparability relations between  $P_i$  and  $P_j$ . Note that  $\hat{\zeta}_C$  is equivalent to the statistic suggested by Rosenbaum [42,43].

In a work on observational studies developed by Gefeller and Pralle [44], it is stated that, what here it is defined as,  $Dom(P_i, P_j)$  and  $Dom(P_j, P_i)$  must fulfil  $Dom(P_i, P_j) + Dom(P_j, P_i) \leq 1$ . This inequality becomes an equality by adding the term of separability between  $P_i$  and  $P_j$ , as in the statement of Theorem 1.

**Corollary 1**  $Dom(P_i, P_j) = Dom(P_j, P_i)$  iff  $T_{j \leq i} = T_{i \leq j}$ .

This corollary states that  $P_i$  dominates  $P_j$  and  $P_j$  dominates  $P_i$  to the same extent only if the number of pairs where  $y \leq x$  is equal to the number of pairs where  $x \leq y$ , having  $x \in P_i$  and  $y \in P_j$ .

Since  $Dom(P_i, P_j)$  depends on the number of comparabilities between  $P_i$  and  $P_j$ , where the elements of  $P_i$  surpass the ones of  $P_j$ , then  $Dom(P_i, P_j)$  can be related to a matrix of comparabilities of this kind.

**Definition 15** Given a Hasse diagram of  $(P, \leq)$ ,  $P_i$  and  $P_j \subset P$  holding  $P_i \cap P_j = \emptyset$ ; then for all  $x \in P_i, y \in P_j$  the indicator function  $M_{xy}^{(i,j)}$  is defined as follows:

$$M_{xy}^{(i,j)} = \begin{cases} 1 & \text{if } y \leq x \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

**Definition 16** Let  $\mathbf{M}^{(i,j)} = [M_{xy}^{(i,j)}]_{n_i \times n_j}$  the matrix representing the  $M_{xy}^{(i,j)}$ -values of  $(x, y) \in P_i \times P_j$ , where  $|P_i| = n_i$  and  $|P_j| = n_j$ .

This matrix can be regarded as an adjacency matrix describing the  $\leq$ -relations among the elements in  $P_i$  and those in  $P_j$ . Note that  $\mathbf{M}^{(i,j)}$  is not a symmetric matrix because of the antisymmetry of  $\leq$  (Definition 2). Since the statistic  $T_{j \leq i}$  (Definition 12) can be derived from this matrix, then  $Dom(P_i, P_j)$  (Definition 13) can also be related to  $\mathbf{M}^{(i,j)}$ .

Each couple of disjoint subsets in  $P$  can be described by an  $\mathbf{M}$  matrix and it is possible to study the relation between subsets by the multiplication of these matrices.

Before describing the meaning of the standard matrix product of  $\mathbf{M}$  matrices, we define the collection of subsets of  $P$  and the  $\leq$ -paths.

**Definition 17** Let  $P$  be a non-empty set and  $\mathbb{P}$  a collection of subsets of  $P$ .  $\mathbb{P}$  partitions  $P$  iff:

1.  $P = \cup_{P_i \in \mathbb{P}} P_i$ ,
2. If  $P_1$  and  $P_2 \in \mathbb{P}$ , then  $P_1 \cap P_2 = \emptyset$ .

**Definition 18** Let  $P_i, P_k, \dots, P_l, P_j \in \mathbb{P}$  and  $r \in P_i, s \in P_k, \dots, t \in P_l, u \in P_j$ . Any sequence of comparabilities  $r \leq s \leq \dots \leq t \leq u$  is called a  $\leq$ -path.

**Proposition 1** Let  $(P, \leq)$  be a poset;  $S \subseteq \mathbb{P}$ ;  $P_i \in S, |P_i| = n_i$ ; and  $G_{\leq}(S)$  the cover graph of  $(S, \leq)$ . Let  $\mathbf{M}^{(i,j)}$  be the associated matrix to any pair  $P_i, P_j \in S$ . Let be the standard matrix product of an arbitrary number of  $\mathbf{M}$  matrices yielding a matrix  $\mathbf{C}$ , defined as follows:  $\mathbf{C}^{(i,j)} = \mathbf{M}^{(i,k)} \cdot \dots \cdot \mathbf{M}^{(l,j)} = [C_{ru}^{(i,j)}]_{n_i \times n_j}$ , with  $i, j$  indicating  $P_i, P_j \in S$  and  $r \in P_i, u \in P_j$ .

If these conditions hold, then each  $C_{ru}^{(i,j)}$  represents the number of  $\leq$ -paths  $r \leq s \leq \dots \leq t \leq u$  between  $r \in P_i$  and  $u \in P_j$  in  $G_{\leq}(S)$  such that these  $\leq$ -paths pass through at least one element of each subset  $P_i, P_k, \dots, P_l, P_j \in S$  considered in the matrix product.



*Proof* We shall prove that given a standard matrix product of  $\mathbf{M}$  matrices, the elements of the final matrix  $\mathbf{C}$  indicate the number of  $\leq$ -paths passing through at least one element of each subset in the matrix product.

Let us start assuming, without loss of generality,  $P = \{a, b, c, d, e, f, g, h\}$  and  $\mathbb{P} = \{P_1, P_2, P_3, P_4\}$  with  $P_1 = \{a, b\}$ ,  $P_2 = \{c, d\}$ ,  $P_3 = \{e, f\}$  and  $P_4 = \{g, h\}$ . Let us consider  $S = \mathbb{P}$  and the following arbitrary  $\mathbf{M}$  matrices.

$$\mathbf{M}^{(1,2)} = \begin{matrix} & c & d \\ a & \begin{bmatrix} M_{ac}^{(1,2)} & M_{ad}^{(1,2)} \\ M_{bc}^{(1,2)} & M_{bd}^{(1,2)} \end{bmatrix} & \\ b & & \end{matrix} \quad \mathbf{M}^{(2,3)} = \begin{matrix} & e & f \\ c & \begin{bmatrix} M_{ce}^{(2,3)} & M_{cf}^{(2,3)} \\ M_{de}^{(2,3)} & M_{df}^{(2,3)} \end{bmatrix} \\ d & & \end{matrix}$$

$$\mathbf{M}^{(3,4)} = \begin{matrix} & g & h \\ e & \begin{bmatrix} M_{eg}^{(3,4)} & M_{eh}^{(3,4)} \\ M_{fg}^{(3,4)} & M_{fh}^{(3,4)} \end{bmatrix} \\ f & & \end{matrix}$$

and their product  $\mathbf{C}^{(1,4)} = \mathbf{M}^{(1,2)} \cdot \mathbf{M}^{(2,3)} \cdot \mathbf{M}^{(3,4)}$

$$\mathbf{C}^{(1,4)} = \begin{matrix} & g & h \\ a & \begin{bmatrix} C_{ag}^{(1,4)} & C_{ah}^{(1,4)} \\ C_{bg}^{(1,4)} & C_{bh}^{(1,4)} \end{bmatrix} \\ b & & \end{matrix} \text{ with}$$

$$C_{ag}^{(1,4)} = M_{ac}^{(1,2)} M_{ce}^{(2,3)} M_{eg}^{(3,4)} + M_{ad}^{(1,2)} M_{de}^{(2,3)} M_{eg}^{(3,4)} + M_{ac}^{(1,2)} M_{cf}^{(2,3)} M_{fg}^{(3,4)} + M_{ad}^{(1,2)} M_{df}^{(2,3)} M_{fg}^{(3,4)}$$

$$C_{ah}^{(1,4)} = M_{ac}^{(1,2)} M_{ce}^{(2,3)} M_{eh}^{(3,4)} + M_{ad}^{(1,2)} M_{de}^{(2,3)} M_{eh}^{(3,4)} + M_{ac}^{(1,2)} M_{cf}^{(2,3)} M_{fh}^{(3,4)} + M_{ad}^{(1,2)} M_{df}^{(2,3)} M_{fh}^{(3,4)}$$

$$C_{bg}^{(1,4)} = M_{bc}^{(1,2)} M_{ce}^{(2,3)} M_{eg}^{(3,4)} + M_{bd}^{(1,2)} M_{de}^{(2,3)} M_{eg}^{(3,4)} + M_{bc}^{(1,2)} M_{cf}^{(2,3)} M_{fg}^{(3,4)} + M_{bd}^{(1,2)} M_{df}^{(2,3)} M_{fg}^{(3,4)}$$

$$C_{bh}^{(1,4)} = M_{bc}^{(1,2)} M_{ce}^{(2,3)} M_{eh}^{(3,4)} + M_{bd}^{(1,2)} M_{de}^{(2,3)} M_{eh}^{(3,4)} + M_{bc}^{(1,2)} M_{cf}^{(2,3)} M_{fh}^{(3,4)} + M_{bd}^{(1,2)} M_{df}^{(2,3)} M_{fh}^{(3,4)}$$

Now, each element  $C_{ag}^{(1,4)}, C_{ah}^{(1,4)}, C_{bg}^{(1,4)}, C_{bh}^{(1,4)}$  of the matrix  $\mathbf{C}^{(1,4)}$  is of the form  $\sum M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$ , with  $r \in P_1, s \in P_2, t \in P_3$  and  $u \in P_4$ .

According to Definition 15, for any  $x \in P_i$  and  $y \in P_j$  with  $P_i \cap P_j = \emptyset$ ,  $M_{xy}^{(i,j)}$  is equal to 1 if  $y \leq x$  and 0 otherwise, therefore each term  $M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$  in  $\sum M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$  is either equal to 1 or to 0. It is 1 if all  $M_{xy}$  have the value 1; that is, if  $r \geq s, s \geq t$  and  $t \geq u$ . It is 0 if at least one  $M_{xy} = 0$ ; that is,

if at least one of these incomparabilities  $r||s, s||t$  or  $t||u$  holds. Hence, each term  $M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$  in  $\sum M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$  indicates if it is possible to find a  $\leq$ -path of the form  $r \geq s \geq t \geq u$  through the particular elements  $r, s, t$  and  $u$ . Consequently,  $\sum M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$  indicates the number of such paths between  $r \in P_1$  and  $u \in P_4$ .

Now, we have to prove that these paths pass through at least one element of the subsets  $P_i$  considered in the matrix product.

Because each  $M_{xy}^{(i,j)}$  always considers only the element  $x$  of  $P_i$  and only the element  $y$  of  $P_j$ , the finding of  $M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)} = 1$  guarantees the existence of a path  $r \geq s \geq t \geq u$  passing exclusively through the elements  $r, s, t$  and  $u$  in the order given by the product. Hence, each element of the matrix  $\mathbf{C}$ , given by  $C_{ru}^{(1,4)} = \sum M_{rs}^{(1,2)} M_{st}^{(2,3)} M_{tu}^{(3,4)}$ , accounts for all the theoretical paths between  $r$  and  $u$  passing through each single element of  $P_s$  and  $P_t$ . Thereby, if  $C_{ru}^{(1,4)} = 0$ , then none of the theoretical paths is realised. In contrast, if  $C_{ru}^{(1,4)} \geq 1$ , the inequality is met if more than one of the theoretical paths between  $r$  and  $u$  passing through single elements of  $P_s$  and  $P_t$  is realised.  $C_{ru}^{(1,4)} = 1$  if at least one of the theoretical paths including single elements of  $P_s$  and  $P_t$  exists.

In conclusion, the  $\leq$ -paths pass through at least one element of the subsets  $P_s$  and  $P_t$ , which are considered in the matrix product.

Because of the properties of the standard matrix product regarding the generality of the elements of a  $\mathbf{C}$  matrix obtained by the finite product of arbitrary  $\mathbf{M}$  matrices, it is possible to extend this result to any finite set  $P$  partitioned into different disjoint subsets gathered in  $\mathbb{P}$  with a subset  $S \subseteq \mathbb{P}$ ;  $S = \{P_1, P_2, P_3, \dots, P_{n-1}, P_n\}$  for which arbitrary matrices are defined in such a way that  $\mathbf{C}^{(i,j)} = \mathbf{M}^{(i,k)} \dots \mathbf{M}^{(l,j)}$ , for any  $P_i, P_k, \dots, P_l, P_j \in S$ . The elements of  $\mathbf{C}^{(i,j)}$  are of the form  $\sum M_{rs} \dots M_{tu}$  with  $r \in P_i, s \in P_k, t \in P_l$  and  $u \in P_j$ . Therefore, each element of  $\mathbf{C}^{(i,j)}$  indicates the number of  $\leq$ -paths passing through at least one element of each subset in the matrix product. □

*Example 2* Let be the Hasse diagram depicted in Fig. 1 and the new subsets  $P_1 = \{a, e\}, P_2 = \{c, d\}$  and  $P_3 = \{g\}$ . In this case there are  $3(3 - 1) = 6$  possible matrices  $\mathbf{M}$ :

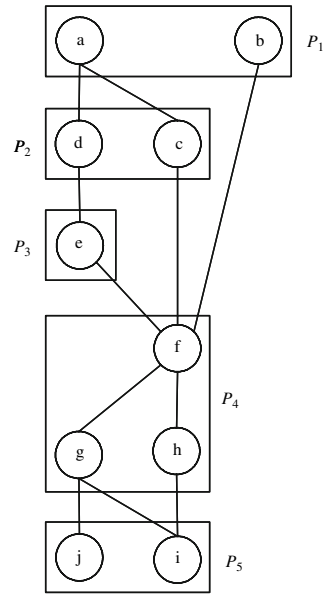
$$\mathbf{M}^{(1,2)} = \begin{matrix} & c & d \\ a & \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \\ e & \end{matrix} \quad \mathbf{M}^{(1,3)} = \begin{matrix} & g \\ a & \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ e & \end{matrix} \quad \mathbf{M}^{(2,1)} = \begin{matrix} a & e \\ c & \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \\ d & \end{matrix}$$

$$\mathbf{M}^{(2,3)} = \begin{matrix} & g \\ c & \begin{bmatrix} 1 \\ 1 \end{bmatrix} \\ d & \end{matrix} \quad \mathbf{M}^{(3,1)} = \begin{matrix} a & e \\ g & \begin{bmatrix} 0 & 0 \end{bmatrix} \end{matrix} \quad \mathbf{M}^{(3,2)} = \begin{matrix} c & d \\ g & \begin{bmatrix} 0 & 0 \end{bmatrix} \end{matrix}$$

If we calculate  $\mathbf{M}^{(1,2)} \cdot \mathbf{M}^{(2,3)}$ , for instance, the matrix  $\mathbf{C}^{(1,3)}$  obtained is:

$$\mathbf{C}^{(1,3)} = \begin{matrix} & g \\ a & \begin{bmatrix} 2 \\ 2 \end{bmatrix} \\ e & \end{matrix}$$

**Fig. 2** A Hasse diagram on the set  $P = \{a, b, c, d, e, f, g, h, i, j\}$ ; four “boxed” subsets  $P_1 = \{a, b\}$ ,  $P_2 = \{c, d\}$ ,  $P_3 = \{e\}$ ,  $P_4 = \{f, g, h\}$  and  $P_5 = \{i, j\}$



The entries of  $C^{(1,3)}$  indicate that there are two  $\leq$ -paths ( $C_{ag}^{(1,3)} = 2$ ) of the form  $g \leq x \leq a$  with  $a \in P_1$ ,  $x \in P_2$  and  $g \in P_3$ ; these two  $\leq$ -paths are  $g \leq c \leq a$  and  $g \leq d \leq a$ . For  $C_{eg}^{(1,3)} = 2$  the corresponding  $\leq$ -paths are  $g \leq c \leq e$  and  $g \leq d \leq e$ . The paths can be easily visualised if the comparability graph of the poset is drawn.

If we consider another product, for example  $M^{(1,3)} \cdot M^{(3,2)}$ , then  $C^{(1,2)} = [0]_{2 \times 2}$  is obtained, which means that there are no possible  $\leq$ -paths of the form  $x \leq g \leq a$ , with  $x \in P_2$ ,  $g \in P_3$  and  $a \in P_1$ , between an element of  $P_1$  and an element of  $P_2$  passing through an element of  $P_3$ .

*Example 3* Let  $P_1 = \{a, b\}$ ,  $P_2 = \{c, d\}$ ,  $P_3 = \{e\}$ ,  $P_4 = \{f, g, h\}$ ,  $P_5 = \{i, j\}$  and the Hasse diagram shown in Fig. 2. In this case there are 20  $M$  matrices; we show 4 of them and their associated  $C^{(1,5)}$  matrix.

$$M^{(1,2)} = \begin{matrix} & c & d \\ a & \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \\ b & \end{matrix} \quad M^{(2,3)} = \begin{matrix} & e \\ c & \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ d & \end{matrix} \quad M^{(3,4)} = \begin{matrix} & f & g & h \\ e & \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \end{matrix} \quad M^{(4,5)} = \begin{matrix} & i & j \\ f & \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 1 & 0 \end{bmatrix} \\ g & \\ h & \end{matrix}$$

$$C^{(1,5)} = M^{(1,2)} \cdot M^{(2,3)} \cdot M^{(3,4)} \cdot M^{(4,5)} = \begin{matrix} & i & j \\ a & \begin{bmatrix} 3 & 2 \\ 0 & 0 \end{bmatrix} \\ b & \end{matrix}$$

Here,  $C_{ai}^{(1,5)} = 3$  which means that there are three  $\leq$ -paths of the form  $i \leq z \leq y \leq x \leq a$  between  $a$  and  $i$  passing through at least one element  $x$  of  $P_2$ , one  $y$  of  $P_3$  and one  $z$  of  $P_4$ ; they are  $i \leq f \leq e \leq d \leq a$ ,  $i \leq g \leq e \leq d \leq a$  and  $i \leq h \leq e \leq d \leq a$ . There are,  $|P_2| \cdot |P_3| \cdot |P_4| = 6$  theoretical paths between  $a$  and  $i$  passing through at

least one element  $x$  of  $P_2$ , one  $y$  of  $P_3$  and one  $z$  of  $P_4$ , the remaining three paths are  $i \leq f \leq e \parallel c \leq a$ ,  $i \leq g \leq e \parallel c \leq a$  and  $i \leq h \leq e \parallel c \leq a$ , which are not possible because of the incomparability  $c \parallel e$ .

## 2.2 Properties of dominance and separability degrees

Once the dominance and separability degrees are calculated, a critical value of dominance or separability may be selected for stating that one subset dominates or is separable from another one. Since dominance degree comes from the total number of possible comparabilities among the elements of the compared subsets, then it is said that the subset  $P_i$  dominates  $P_j$ , when more than half of the possible relations among the elements of  $P_i$  and  $P_j$  are comparabilities  $y \leq x$  with  $x \in P_i$  and  $y \in P_j$ . Thus, we are interested in values of  $Dom(P_i, P_j) > 0.5$ , which, according to Theorem 1, guarantees that  $Dom(P_j, P_i) + Sep(P_i, P_j) < 0.5$ ; for that reason if  $Dom(P_i, P_j) > 0.5$  then,  $P_j$  cannot dominate  $P_i$ . The limiting value for  $Dom(P_i, P_j)$  could also be shifted to high scores, for example 0.9, in which case we look for subsets  $P_i$  and  $P_j$  for which 90% of the possible relations among elements of  $P_i$  and  $P_j$  are comparabilities where  $y \leq x$  with  $x \in P_i$  and  $y \in P_j$ .

**Definition 19** We say  $P_i$   $\varepsilon$ -dominates  $P_j$  iff  $Dom(P_i, P_j) > \varepsilon$  with  $\varepsilon \in [0.5, 1)$ . In that case it is written  $P_j \prec_\varepsilon P_i$ .

It is important to note the meaning of  $Dom(P_i, P_j) > \varepsilon$  with  $\varepsilon \in [0.5, 1)$ . It implies to have dominance degree values greater than an  $\varepsilon$  in the interval  $[0.5, 1)$ , which means to have dominance degree values in the interval  $(0.5, 1]$ .

In order to explore the properties of  $\prec_\varepsilon$ , we display six general properties of binary relations.

**Definition 20** Let  $X \neq \emptyset$  and  $R$  a binary relation on  $X$ . Then six possible properties of  $R$  are:

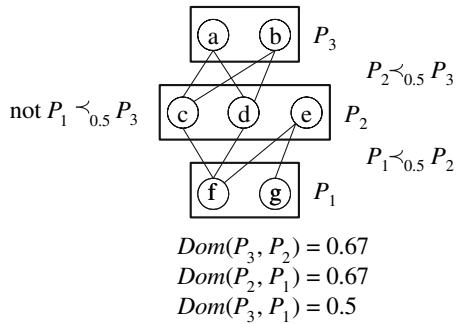
1.  $x \in X \Rightarrow xRx$  (reflexive),
2.  $x \in X \Rightarrow \text{not } xRx$  (irreflexive),
3.  $x, y \in X, xRy \Rightarrow yRx$  (symmetric),
4.  $x, y \in X, xRy \Rightarrow \text{not } yRx$  (asymmetric),
5.  $x, y \in X, xRy$  and  $yRx \Rightarrow x = y$  (antisymmetric),
6.  $x, y, z \in X, xRy$  and  $yRz \Rightarrow xRz$  (transitive).

**Proposition 2** From the properties shown in Definition 20,  $\prec_\varepsilon$  is only irreflexive and asymmetric on  $P$ .

*Proof* 1, 2.  $\prec_\varepsilon$  is irreflexive and not reflexive because it is a binary relation defined on  $P$ , whose elements are disjoint subsets (Definition 17).

3. If  $\prec_\varepsilon$  is to be a symmetric relation, then  $P_j \prec_\varepsilon P_i \Rightarrow P_i \prec_\varepsilon P_j$ , with  $P_i, P_j \in P$ . If  $P_j \prec_\varepsilon P_i$ , then, from Definition 13,  $T_{j \leq i} > \varepsilon(n_i \cdot n_j)$ . According to Theorem 1, the maximum number of  $x \leq y$  relations, for all  $x \in P_i$  and  $y \in P_j$ , is given by  $T_{j \leq i} + T_{i \leq j} = n_i \cdot n_j (T_{i \parallel j} = 0)$ . Knowing that  $T_{j \leq i} > \varepsilon(n_i \cdot n_j)$  then  $T_{i \leq j} < n_i \cdot n_j(1 - \varepsilon)$ . Hence,  $T_{i \leq j}$  not  $> \varepsilon(n_i \cdot n_j)$ , therefore  $P_i$  not  $\prec_\varepsilon P_j$ .

**Fig. 3** A Hasse diagram showing the lack of transitivity of  $<_{\varepsilon}$



4. If  $<_{\varepsilon}$  is asymmetric then  $P_j <_{\varepsilon} P_i \Rightarrow \text{not } P_i <_{\varepsilon} P_j$  as was shown before (3).

5. In order to prove that  $<_{\varepsilon}$  is not antisymmetric, let  $P_i, P_j \in \mathbb{P}$  and  $n_i = |P_i|, n_j = |P_j|$ . The two initial conditions of the antisymmetry are  $P_j <_{\varepsilon} P_i$  and  $P_i <_{\varepsilon} P_j$ . It is enough to prove that they cannot be given simultaneously in  $\mathbb{P}$ . If  $P_j <_{\varepsilon} P_i$  then, from Theorem 1,  $T_{j \leq i} > (T_{i \leq j} + T_{i || j})$ ; if  $P_i <_{\varepsilon} P_j$  then  $T_{i \leq j} > (T_{j \leq i} + T_{i || j})$ ; thereby  $T_{i || j} < T_{j \leq i} - T_{i \leq j} < -T_{i || j}$ , which is a contradiction and  $P_j <_{\varepsilon} P_i, P_i <_{\varepsilon} P_j$  cannot hold simultaneously.

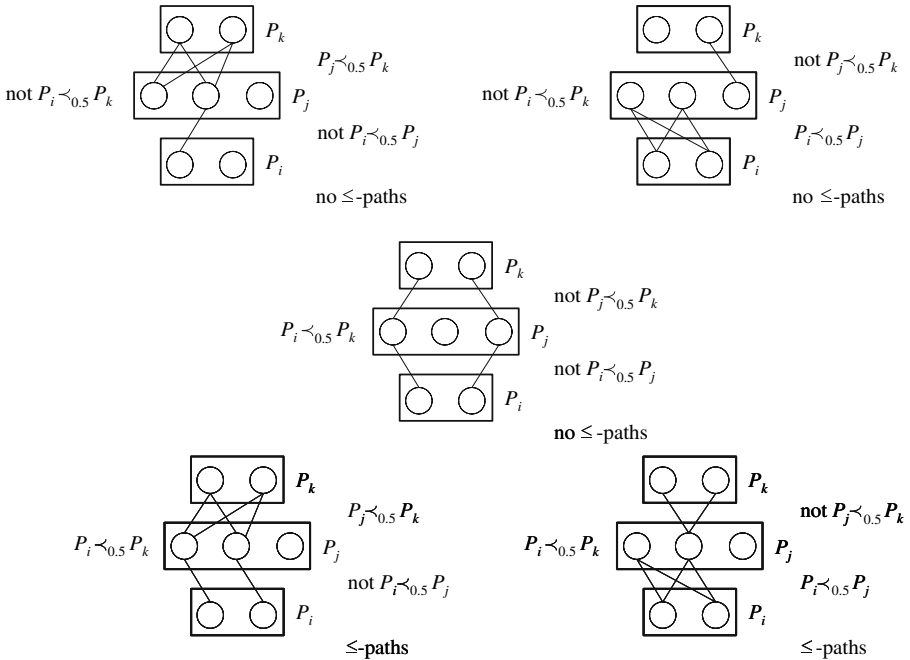
6. An example showing the lack of transitivity of  $<_{\varepsilon}$  is illustrated in Fig. 3.  $P_j <_{\varepsilon} P_i$  means  $\text{Dom}(P_i, P_j) > \varepsilon$  with  $\varepsilon \in [0.5, 1)$ . In this example (Fig. 3),  $\text{Dom}(P_3, P_2), \text{Dom}(P_2, P_1) > 0.5$ , then  $P_2 <_{0.5} P_3$  and  $P_1 <_{0.5} P_2$  but  $\text{Dom}(P_3, P_1) = 0.5$ , therefore not  $P_1 <_{0.5} P_3$ . □

If we consider again the Hasse diagram of Fig. 3 and we add to it the comparability  $g \leq d$ , it keeps holding  $P_2 <_{0.5} P_3$  and  $P_1 <_{0.5} P_2$  but now  $P_1 <_{0.5} P_3$ , in fact  $\text{Dom}(P_3, P_1) = 1$ . Why does it occur? Because  $g \leq d$  permits the additional comparabilities  $g \leq a$  and  $g \leq b$ . On the other hand  $P_2 <_{0.5} P_3$  and  $P_1 <_{0.5} P_2$  are maintained together with  $P_1 <_{0.5} P_3$  because more than half of the relations among elements of  $P_3$  and  $P_1$  correspond to  $x \leq y \leq z$ , where  $x \in P_1, y \in P_2$  and  $z \in P_3$ . It is, more than half of the pairs  $x, z$  are related by a  $\leq$ -path  $x \leq y \leq z$  passing through some element of  $P_2$ . Then, the existence of these paths is determinant for the  $\leq$ -relation of two subsets having a third one in between.

The above statement makes one think that  $<_{\varepsilon}$  may become a transitive relation if it is endowed with  $\leq$ -paths. That is correct but then the transitivity is not a property of  $<_{\varepsilon}$ , as we show in Proposition 2, but of the structure  $(<_{\varepsilon}, \leq\text{-paths})$ .

In Fig. 4 we show five Hasse diagrams, three subposets, and their dominance relations for  $\varepsilon = 0.5$ ; additionally we show the presence or absence of  $\leq$ -paths between those subposets. We write no  $\leq$ -paths (Fig. 4) if the number of  $\leq$ -paths  $x \leq y \leq z$  between  $P_i$  and  $P_k$  is less than or equal than half of  $n_i \cdot n_k$ .

From the Hasse diagrams shown in Fig. 4 and from the discussion about Fig. 3, it can be concluded that always the presence of more than  $(n_i \cdot n_k)/2$   $\leq$ -paths  $x \leq y \leq z$  guarantees that  $P_i <_{0.5} P_k$ . However, those  $\leq$ -paths alone are not a guarantee of  $P_i <_{0.5} P_j$  and  $P_j <_{0.5} P_k$ . Then, in order to have an implication similar to  $P_i <_{0.5} P_j, P_j <_{0.5} P_k \Rightarrow P_i <_{0.5} P_k$ , it is necessary to meet  $P_i <_{0.5} P_j, P_j <_{0.5} P_k$



**Fig. 4** Four Hasse diagrams,  $<_{0.5}$  relations for its subsets and the presence/absence of  $\leq$ -paths among them

and to guarantee the existence of more than  $(n_i \cdot n_k)/2$   $\leq$ -paths of the form  $x \leq y \leq z$  with  $x \in P_i, y \in P_j$  and  $z \in P_k$ .

**Theorem 2** Let  $P_i, P_j, P_k \in P$  such that there are more than  $\varepsilon(n_i \cdot n_k)$   $\leq$ -paths of the sort  $x \leq y \leq z$ , with  $x \in P_i, y \in P_j$  and  $z \in P_k$ , and  $P_i <_{\varepsilon} P_j, P_j <_{\varepsilon} P_k$ . If this is satisfied, then  $P_i <_{\varepsilon} P_k$ .

*Proof*  $P_i <_{\varepsilon} P_j$  ensures that there are more than  $\varepsilon(n_i \cdot n_j)$  relations  $x \leq y$  with  $x \in P_i, y \in P_j$ . In the same way  $P_j <_{\varepsilon} P_k$  guarantees the existence of more than  $\varepsilon(n_j \cdot n_k)$  relations  $y \leq z$  with  $z \in P_k$ . Since  $\varepsilon \in [0.5, 1)$ , then both  $P_i <_{\varepsilon} P_j$  and  $P_j <_{\varepsilon} P_k$  ensure the existence of at least one  $\leq$ -path  $x \leq y \leq z$ . If there are more than  $\varepsilon(n_i \cdot n_k)$   $\leq$ -paths  $x \leq y \leq z$ , then  $T_{i \leq k} > \varepsilon(n_i \cdot n_k)$ , thereby  $Dom(P_k, P_i) > \varepsilon$  and  $P_i <_{\varepsilon} P_k$ . It is, the number of  $\leq$ -paths required to state  $P_i <_{\varepsilon} P_k$  depend on  $n_i$  and  $n_k$  but not on  $n_j$ . Because of this, from the number of these  $\leq$ -paths cannot be inferred if  $T_{j \leq k} > \varepsilon(n_j \cdot n_k)$  neither if  $T_{i \leq j} > \varepsilon(n_i \cdot n_j)$ ; or in other words whether  $P_j <_{\varepsilon} P_k$  or not. The inclusion of  $P_j <_{\varepsilon} P_k$  and  $P_i <_{\varepsilon} P_j$  as additional conditions of this theorem then are a guarantee that  $P_i <_{\varepsilon} P_k$  □

**Definition 21** Two sets  $P_i, P_j \in P$  are said to be  $\varepsilon$ -dominable iff either  $P_i <_{\varepsilon} P_j$  or  $P_j <_{\varepsilon} P_i$ . We say that  $P_i$   $\varepsilon$ -dominates  $P_j$  if  $P_j <_{\varepsilon} P_i$ .

**Definition 22** Given two sets  $P_i, P_j \in P$ , we say that  $P_i$  is covered by  $\varepsilon$ -dominance by  $P_j$ , denoted  $P_i <_{\varepsilon}: P_j$ , if  $P_i <_{\varepsilon} P_j$  and there is no  $P_k \in P$  for which  $P_i <_{\varepsilon} P_k$  and  $P_k <_{\varepsilon} P_j$ . If  $P_i <_{\varepsilon}: P_j$ , it is said that  $P_j$  covers by  $\varepsilon$ -dominance  $P_i$ .

**Definition 23** Given  $P_i, P_j \in \mathbb{P}$ , it is said that  $P_i$  is  $\delta$ -separated from  $P_j$  or  $P_j$  is  $\delta$ -separated from  $P_i$  iff  $Sep(P_i, P_j) > \delta$  with  $\delta \in [0.5, 1)$ . In that case it is written  $P_i \parallel_\delta P_j$  and we say that  $P_i$  and  $P_j$  are  $\delta$ -separable.

**Proposition 3** From the properties shown in Definition 20,  $\parallel_\delta$  is irreflexive and symmetric on  $\mathbb{P}$ .

*Proof* 1, 2. The relation  $\parallel_\delta$  is irreflexive because the elements of  $\mathbb{P}$  are mutually disjoint subsets; for the same reason it is not reflexive.

3, 4.  $\parallel_\delta$  is symmetric by definition since  $Sep(P_i, P_j) = Sep(P_j, P_i)$  (Definition 13); hence it is not asymmetric.

5. Although  $P_i \parallel_\delta P_j$  and  $P_j \parallel_\delta P_i$  can always coexist, it does not imply that  $P_i = P_j$  because  $P_i \cap P_j = \emptyset$ , then  $\parallel_\delta$  is not antisymmetric.

6. In order to show the no transitivity of  $\parallel_\delta$ , let us assume that the poset in Fig. 3 is an incomparability graph (Definition 10), then each link in it is a  $\parallel_\delta$  relation where it holds  $P_1 \parallel_\delta P_2, P_2 \parallel_\delta P_3$  but not  $P_1 \parallel_\delta P_3$ . Therefore  $\parallel_\delta$  is not a transitive relation on  $\mathbb{P}$ . □

Then  $\parallel_\delta$  is defined as follows:

**Definition 24** The  $\delta$ -separability relation  $\parallel_\delta$  is a binary relation on  $\mathbb{P}$  fulfilling these properties:

1.  $P_i \in \mathbb{P} \Rightarrow \text{not } P_i \parallel_\delta P_i,$
2.  $P_i, P_j \in \mathbb{P}, P_i \parallel_\delta P_j \Rightarrow P_j \parallel_\delta P_i.$

**Definition 25** Let  $G_{<_\varepsilon} = (\mathbb{P}, E_{<_\varepsilon})$  the  $\varepsilon$ -dominance graph, where  $E_{<_\varepsilon}$  is the set of edges containing all the  $\varepsilon$ -dominable pairs in  $\mathbb{P}$ .

**Definition 26** Let  $G_{\parallel_\delta} = (\mathbb{P}, E_{\parallel_\delta})$  the  $\delta$ -separability graph, where  $E_{\parallel_\delta}$  is the set of edges containing all the  $\delta$ -separable pairs in  $\mathbb{P}$ .

**Definition 27** Let  $G_{<_\varepsilon} = (\mathbb{P}, E_{<_\varepsilon})$  the cover by  $\varepsilon$ -dominance graph, where  $E_{<_\varepsilon}$  is the set of edges containing all the cover by  $\varepsilon$ -dominance pairs in  $\mathbb{P}$ .

In general, because of the lack of transitivity of  $<_\varepsilon$  it is not possible to associate a Hasse diagram to  $\mathbb{P}$ , but if the comparabilities and incomparabilities among the elements of  $\mathbb{P}$  permit the existence of  $\leq$ -paths, as described in Theorem 2, then a Hasse diagram on the elements of  $\mathbb{P}$  can be drawn.

**Definition 28** Let  $H = (\mathbb{P}, d(E_{<_\varepsilon}))$  a directed graph of  $(\mathbb{P}, <_\varepsilon, C)$  where  $d(E_{<_\varepsilon})$  is the set of directed edges containing the cover by  $\varepsilon$ -dominance pairs in  $\mathbb{P}$ .  $H$  is called the  $\varepsilon$ -dominance Hasse diagram of the structure  $(\mathbb{P}, <_\varepsilon, C)$ , where  $C$  is the collection of  $\leq$ -paths described in Theorem 2, if  $H$  is drawn in the Euclidean plane whose horizontal/vertical coordinate system requires that the vertical coordinate of  $P_i \in \mathbb{P}$  be larger than the one of  $P_j \in \mathbb{P}$  if  $P_j <_\varepsilon P_i$ .

### 3 Application to chemical posets

#### 3.1 Ordering molecular total energies of isoelectronic species with equal total nuclear charge

The molecular total energy  $E(Z, R)$  can be considered as a function of the nuclear geometry  $R$  and the nuclear charges  $Z$  in such a way that energy relations for different molecular species can be reached by variations of  $R$  and  $Z$ . By energy relations Mezey [45], Villaveces, Daza and Bernal [32, 33, 46] refer to order relationships between the total energy of molecular species. However,  $E(Z, R)$  is mathematically complicated and it is usual to restrict the study of such relationships to particular cases of  $R$  and  $Z$ , e.g.  $Z$  fixed while  $R$  changes and  $R$  fixed while  $Z$  changes, both cases considering isoelectronic species [45]. The constraint of  $R$  fixed and  $Z$  variable, together with the Born-Oppenheimer approximation has led to obtain general expressions showing order relationships between total energies of isoelectronic molecular species [32]. This kind of studies were initiated by Thirring, Narnhofer, Lieb and Simon [47–49] in the 1970s and further extended by Mezey in the 1980s [45, 50–53]. Villaveces, Daza and Bernal [32, 33, 46] have generalised these ideas and have developed elegant theorems to order isoelectronic molecular species in their minimum energy configurations. A brief description of these results is given as follows.

Two isoelectronic species  $Z^{(A)}$  and  $Z^{(B)}$  with equal total nuclear charge  $N$  are called *isoelectronic–isoprotonic species* and are represented by nuclear charge vectors  $Z^{(A)} = (Z_1^{(A)}, Z_2^{(A)}, \dots, Z_N^{(A)})$  and  $Z^{(B)} = (Z_1^{(B)}, Z_2^{(B)}, \dots, Z_N^{(B)})$ , respectively, where  $Z_i^{(k)}$  is the  $i$ -th component of the vector  $k$ , which corresponds to the  $i$ -th nucleus in the species  $k$ .

A set  $S$  of vectors in “general position” [46] constitutes the vertices of a polyhedron  $P(S)$  in the space of isoelectronic–isoprotonic species. An example of vectors in general position is constituted by the atomic vectors  $(N, 0, 0, \dots, 0)$ ,  $(0, N, 0, \dots, 0)$ ,  $\dots$ ,  $(0, 0, 0, \dots, N)$ , which are atomic vectors of nuclear charge  $N$ . In general,  $S = \{Z^{(1)}, Z^{(2)}, \dots, Z^{(p)}\}$  and the polyhedron is defined as

$$P(S) = \left\{ Z : Z = \sum_{k=1}^p \alpha_k Z^{(k)}, Z^{(k)} \in S, \sum_{k=1}^p \alpha_k = 1, \alpha_k \geq 0, \right. \\ \left. k = 1, 2, \dots, p \right\} \quad (7)$$

$P(S)$  contains all the isoelectronic–isoprotonic species that can be generated by linear combinations of isoelectronic–isoprotonic atomic vectors, if these vectors are selected as the generating vertices of the polyhedron.

The Born-Oppenheimer, BO, operator that generates the BO molecular total energy of any isoelectronic–isoprotonic species in the polyhedron can be expressed in terms of polyhedron vertices when all molecules in such a polyhedron hold the same nuclear configuration  $R$ . This energy is bounded by:

$$E_R(Z) \geq \sum_k^p \alpha_k E_R(Z^{(k)}) + Q \quad (8)$$



where  $Q$  depends on the vertices generating the polyhedron. If  $Q \geq 0$ , it can be removed from the inequality without altering it. It has been shown [32] that a set of  $Z^{(k)}$ 's yielding  $Q \geq 0$  is a subset  $S_a$  of vertices, in which any two of them can be obtained by permutations of its components. Additionally, these permutations must be equal to a product of disjoint transpositions (details are given in Refs [32,33]).

In general, if the minimum energy configurations of two isoelectronic–isoprotonic species  $Z$  and  $Z^{(i)}$  are selected, and if  $Z$  can be obtained by permuting components of  $Z^{(i)}$ , then the following inequality holds [32,33]:

$$\min_R E(Z) \geq \min_R E(Z^{(i)}) \quad (9)$$

Hence, the BO molecular total energy of any two isoelectronic–isoprotonic species  $Z^{(A)}$  and  $Z^{(B)}$  in their minimum energy configurations can be ordered and one of these two order relations may result:

$$\min_R E(Z^{(A)}) \geq \min_R E(Z^{(B)}) \quad (10)$$

$$\min_R E(Z^{(B)}) \geq \min_R E(Z^{(A)}) \quad (11)$$

To check if Eq. 10 holds, the set of permutations of  $Z^{(B)}$  is obtained, that is  $S_B = \{Z^{(B)1}, Z^{(B)2}, \dots, Z^{(B)p}\}$ . If  $Z^{(A)}$  belongs to the polyhedron generated by  $S_B$ , then Eq. 10 is satisfied. In particular, this implies to solve the following set of linear equations:

$$\begin{aligned} Z_1^{(A)} &= \sum_i^p \alpha_i Z_1^{(B)i} \\ Z_2^{(A)} &= \sum_i^p \alpha_i Z_2^{(B)i} \\ &\vdots \\ Z_N^{(A)} &= \sum_i^p \alpha_i Z_N^{(B)i} \end{aligned} \quad (12)$$

Thus, if each component of  $Z^{(A)}$  is actually generated by linear combinations of vectors obtained by permutations of components of  $Z^{(B)}$ , then the BO molecular total energy of  $Z^{(A)}$  is higher than the one of  $Z^{(B)}$  in their minimum energy configurations. If it is not possible to solve the linear equations, then the other possibility (Eq. 11) must be tested. If none of these sets of linear equations can be solved, then it is said that the BO molecular total energies of  $Z^{(A)}$  and  $Z^{(B)}$  in their minimum energy configurations are incomparable. In that case it may be written

$$\min_R E(Z^{(A)}) \parallel \min_R E(Z^{(B)}) \quad (13)$$

In the following we apply the dominance and separability degrees to the BO molecular total energies of the complete set of isoelectronic–isoprotonic species with total nuclear charge 10.

### 3.2 Molecular total energies of isoelectronic–isoprotonic species with total nuclear charge 10

The Hasse diagram of the set  $P$  of BO molecular total energies of 42 isoelectronic–isoprotonic species with charge 10 was recently published by Daza and Bernal [32,33] (Fig. 5). In this diagram, objects holding high and low energies are respectively located at the top and bottom of the diagram. We partition  $P$  into 10 subsets containing, each one, all the objects with same number of nuclei; these subsets are:  $P_1 = \{\text{Ne}\}$ ,  $P_2 = \{\text{HF}, \text{HeO}, \text{NLi}, \text{CBe}, \text{B}_2\}$ ,  $P_3 = \{\text{H}_2\text{O}, \text{NHeH}, \text{CLiH}, \text{CHe}_2, \text{BBeH}, \text{BLiHe}, \text{Be}_2\text{He}, \text{BeLi}_2\}$ ,  $P_4 = \{\text{NH}_3, \text{CHeH}_2, \text{BLiH}_2, \text{BHe}_2\text{H}, \text{Be}_2\text{H}_2, \text{BeLiHeH}, \text{BeHe}_3, \text{Li}_3\text{H}, \text{Li}_2\text{He}_2\}$ ,  $P_5 = \{\text{CH}_4, \text{BHeH}_3, \text{BeLiH}_3, \text{BeHe}_2\text{H}_2, \text{Li}_2\text{HeH}_2, \text{LiHe}_3\text{H}, \text{He}_5\}$ ,  $P_6 = \{\text{BH}_5, \text{BeHeH}_4, \text{Li}_2\text{H}_4, \text{LiHe}_2\text{H}_3, \text{He}_4\text{H}_2\}$ ,  $P_7 = \{\text{BeH}_6, \text{LiHeH}_5, \text{He}_3\text{H}_4\}$ ,  $P_8 = \{\text{LiH}_7, \text{He}_2\text{H}_6\}$ ,  $P_9 = \{\text{HeH}_8\}$  and  $P_{10} = \{\text{H}_{10}\}$ . Hence,  $P = \{P_i : i = 1, 2, \dots, 10\}$ .

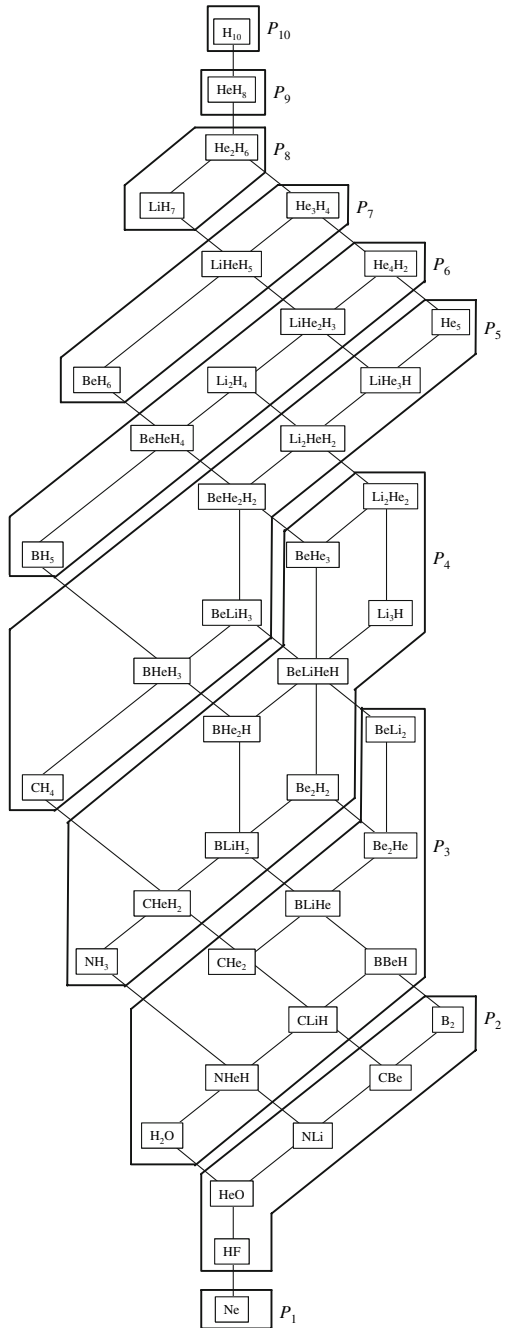
This Hasse diagram, in fact a lattice, shows  $P_{10} = \{\text{H}_{10}\}$  as the maximal subset, it is that the hydrogen cluster has the maximum BO energy of all the isoelectronic–isoprotonic species with total nuclear charge 10. In contrast, the minimal subset is  $P_1 = \{\text{Ne}\}$ , it is the Neon atom. Hence, the BO energies of all the isoelectronic–isoprotonic species in their minimum energy configurations with total nuclear charge 10 are in-between the energy of Ne and  $\text{H}_{10}$ . This result has been mathematically formalised and generalised by Daza and Bernal [32,33] to any set of isoelectronic–isoprotonic species in their minimum energy configurations.

From the total of 100 ordered pairs  $(P_i, P_j) \in P \times P$ , the dominance and separability degrees are defined for 90 of them because of the condition of having disjoint subsets (Definitions 14 and 15). Thus, for each one of the 45 sets  $\{P_i, P_j\}$  (non-ordered pairs) the parameters  $Dom(P_i, P_j)$ ,  $Dom(P_j, P_i)$  and  $Sep(P_i, P_j)$  were calculated (Table 1).

It is particularly interesting to note that  $Dom(P_i, P_j) = 0$  and  $Dom(P_j, P_i) > Sep(P_i, P_j)$  in all the cases, then any comparison of two subsets  $P_i$  and  $P_j$ , where  $P_i$  contains objects with fewer nuclei than  $P_j$ , shows that  $P_i <_{\varepsilon} P_j$ , and because  $Dom(P_i, P_j) = 0$  then there are no cases where a species  $x$  having fewer nuclei than another  $y$  has more energy than  $y$  as has been proved by Daza and Bernal [32,33].

From Table 1 it can be seen that 66.7% of the pairs  $\{P_i, P_j\}$  correspond to the complete dominance of  $P_j$  over  $P_i$ , it is  $Dom(P_j, P_i) = 1$  and  $Sep(P_i, P_j) = 0$ . These dominance and separability values are related by  $P_i <_{\varepsilon} P_j$ , with  $\varepsilon$  taking all the possible values in the real interval  $(0.5, 1]$ . Additionally, these subsets do not present incomparabilities between their members, meaning that all the species in  $P_j$  have higher BO energies than all the species in  $P_i$ . This situation occurs for pairs of subsets located up and down in the Hasse diagram, for instance  $P_8$  and  $P_2$ . The maximum values of separability degrees occur for adjacent pairs of subsets holding the highest number of incomparable BO energies between their objects, the pair of subsets with maximum separability is  $P_5, P_6$  ( $Sep(P_5, P_6) = 0.31$ ). Although this is the maximum separability degree value it cannot be stated that  $P_5 ||_{\delta} P_6$  because the condition  $Sep(P_5, P_6) > 0.5$  does not hold.

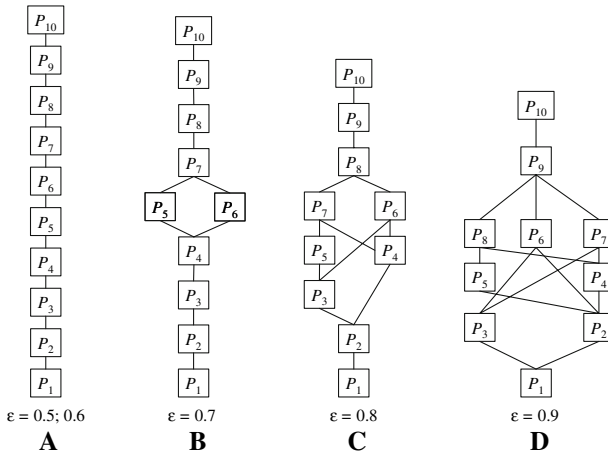
**Fig. 5** Hasse diagram of the 42 isoelectronic species with total nuclear charge 10. The boxes represent species with same number of nuclei



**Table 1** Dominance and separability degrees for 10 subsets of the Hasse diagram depicted in Fig. 5

| $\{P_i, P_j\}^a$   | $Dom(P_i, P_j)$ | $Dom(P_j, P_i)$ | $Sep(P_i, P_j)$ |
|--|-----------------|-----------------|-----------------|
| $\{1,2\},\{1,3\},\{1,4\},\{1,5\},\{1,6\},\{1,7\},\{1,8\},\{1,9\},\{1,10\},\{2,6\},\{2,7\},\{2,8\},\{2,9\},\{2,10\},\{3,7\},\{3,8\},\{3,9\},\{3,10\},\{4,8\},\{4,9\},\{4,10\},\{5,9\},\{5,10\},\{6,9\},\{6,10\},\{7,9\},\{7,10\},\{8,9\},\{8,10\},\{9,10\}$ | 0               | 1               | 0               |
| $\{2,5\}$  | 0               | 0.97            | 0.03            |
| $\{3,6\}$  | 0               | 0.95            | 0.05            |
| $\{2,4\},\{4,7\},\{5,8\}$  | 0               | 0.93            | 0.07            |
| $\{6,8\}$  | 0               | 0.9             | 0.1             |
| $\{3,5\}$  | 0               | 0.89            | 0.11            |
| $\{4,6\}$  | 0               | 0.84            | 0.16            |
| $\{2,3\},\{7,8\}$  | 0               | 0.83            | 0.17            |
| $\{5,7\}$  | 0               | 0.81            | 0.19            |
| $\{3,4\}$  | 0               | 0.79            | 0.21            |
| $\{4,5\},\{6,7\}$  | 0               | 0.73            | 0.27            |
| $\{5,6\}$  | 0               | 0.69            | 0.31            |

<sup>a</sup> We renamed the set  $P_i$  and  $P_j$  as  $i$  and  $j$ , respectively



**Fig. 6** (A) 0.5–, 0.6–; (B) 0.7–; (C) 0.8– (D) 0.9-dominance Hasse diagrams of the subsets remarked in Fig. 5

Since the structure of the Hasse diagram guarantees the existence of  $\leq_\epsilon$ -paths of the sort discussed in Theorem 2, it is possible to draw  $\epsilon$ -dominance Hasse diagrams for  $(P, <_\epsilon, C)$ . We show in Fig. 6 four  $\epsilon$ -dominance Hasse diagrams

Different  $\epsilon$ -values yield different kinds of information regarding the comparabilities among the considered subsets. In general low  $\epsilon$ -values give a broad landscape of the order relations and high  $\epsilon$ -values permit going into the details of the relations. For example, the diagram A (Fig. 6) shows dominance degree values greater than 0.5 and also greater than 0.6; from its linear order it can be concluded that a direct relationship between the BO energies and the number of nuclei in the species holds for these

levels of dominance degrees. Using the dominance degree values it can be found the maximum value of  $\varepsilon$  for which the linear order of Fig. 6A holds. In this case the linear order is kept only up to values of dominance degree equal or less than 0.7 (Fig. 6B); this result can be interpreted as: given two subsets  $P_i$  and  $P_j$  containing, respectively, species with  $i$  and  $j$  nuclei ( $i > j$ ), then at least 70% of the pairs  $(x, y) \in P_i \times P_j$  holds that the energy of  $x$  is higher than the energy of  $y$ .

Additionally, the possibility of varying  $\varepsilon$  allows adjusting the level of detail we want to explore concerning the order relations; for instance, if  $\varepsilon = 0.7$ , then  $P_6$  and  $P_5$  become incomparable. That is, when we look for subsets where more than 70% of the pairs  $(x, y) \in P_i \times P_j$  holds that the energy of  $x$  is higher than the energy of  $y$ , then  $P_6$  and  $P_5$  are not regarded because of their incomparability (not  $P_5 <_{0.7} P_6$ ), it means that no more than 70% of the pairs  $(x, y) \in P_6 \times P_5$  holds that the energy of  $x$  is higher than the one of  $y$ .

If  $\varepsilon$  is shifted to  $\varepsilon = 0.8$  then more subsets become incomparable (Fig. 6C) and it can be seen that they start to appear around  $P_5$  and  $P_6$  (the subsets having more incomparabilities per total relations). At this level of dominance degree the following relations can be seen:  $P_3 <_{0.8} P_5 <_{0.8} P_7$ ,  $P_2 <_{0.8} P_4 <_{0.8} P_6 <_{0.8} P_8$ . In general a subset  $P_i$  in  $\{P_2, P_3, \dots, P_8\}$  dominates  $P_{i-2}$  in  $\{P_2, P_3, \dots, P_8\}$ . This mainly occurs because the least energetic species in  $P_i$  is able to dominate more than 80% of the species in  $P_{i-2}$  but not more than 80% of the objects in  $P_{i-1}$ . This is the case for  $\text{BeH}_6$ ,  $\text{BH}_5$ ,  $\text{CH}_4$  and  $\text{NH}_3$ .

Fig. 6D shows the 0.9-dominance Hasse diagram, and it presents those subsets for which more than 90% of their species present more BO energies than others in different subsets. In general the amount of incomparabilities increase showing that the linear order depicted in Fig. 6A is in fact caused by the low level of dominance considered in that case ( $\varepsilon = 0.5, 0.6$ ).

Now if we consider high  $\varepsilon$ -values and compare the corresponding  $\varepsilon$ -diagrams with the ones of low  $\varepsilon$ -values, it can be seen that the dominances present in the diagram with high  $\varepsilon$ -values are kept in the diagrams of low  $\varepsilon$ -values, for example  $P_3 <_{\varepsilon} P_7$  in all the diagrams shown in Fig. 6. This relation between Hasse diagrams is known as order preserving, in this case dominances present in high  $\varepsilon$ -dominance Hasse diagrams are preserved in the diagrams of low  $\varepsilon$ -values. Formally, given  $\varepsilon > \varepsilon'$ , the mapping  $(P, <_{\varepsilon}, C) \rightarrow (P, <_{\varepsilon'}, C)$ ,  $<_{\varepsilon'} C <_{\varepsilon}$  is order preserving if any  $P_i <_{\varepsilon} P_j \in (P, <_{\varepsilon}, C)$  implies  $P_i <_{\varepsilon'} P_j \in (P, <_{\varepsilon'}, C)$ .

The incomparabilities between subsets that begin to be prominent for  $\varepsilon$  greater than 0.7, occur because of the distribution of the comparabilities among the objects in the subposet, as expected. All the relations among subsets (Fig. 5), except those between  $P_{10}$ ,  $P_9$ ,  $P_2$  and  $P_1$  are characterised (1) for the surpassing of a high energetic species of  $P_j$  over all the species of  $P_i$ , where  $P_j$  contains objects with more nuclei than those in  $P_i$ ; and (2) for the surpassing of the lowest energetic species of  $P_j$  over the 2 lowest energetic species of  $P_i$ . An example of (1) is the surpassing of  $\text{He}_3\text{H}_4 \in P_7$  over all the objects in  $P_6$  and an example of (2) is the surpassing of  $\text{CH}_4 \in P_5$  only over  $\text{CHeH}_2$  and  $\text{NH}_3$ , which belong to  $P_4$ . A remark extracted from 2) is that the deletion of the least energetic object of the subsets  $P_8$  to  $P_3$  would strengthen the dominance relations between the subsets and this effect would be especially notorious for high BO energy subsets. For example, the effect of removing  $\text{LiH}_7$  in  $P_8$  (a high BO energy

subset) would cause that  $Dom(P_8, P_7)$  change from 0.83 to 1 and the effect of deleting  $H_2O$  in  $P_3$  (a low BO energy subset) would shifted  $Dom(P_3, P_2)$  just from 0.83 to 0.89. This study opens the possibility of determining the most influent species for the dominance of their respective subsets when compared with others.

Regarding the separability degree results (Table 1), they are not a determining structural factor of the diagrams depicted in Fig. 6 because of their low values. According to Theorem 1, these separability degree values are compensated for the high results of dominance degree which in turn yield many  $\varepsilon$ -dominances in the  $\varepsilon$ -dominance Hasse diagrams.

## 4 Conclusion and outlook

In this paper we present the mathematical background of a methodology that permits to draw conclusions on the relations of comparabilities and incomparabilities between pairs of disjoint subposets in  $(P, \leq)$ . Particularly, the dominance degree measures the extent of comparabilities in the considered subsets while the separability degree considers the corresponding incomparabilities. An advantage of this method over the analysis of the poset of class-representatives after clustering the elements in  $P$  is that the method here presented does not reduce the cardinality of the ground set  $P$  of the original poset, therefore all the relations between all the pairs of the two compared subsets are considered. It is, the dominance and separability of two subposets is assessed by evaluating all the elements of both subposets and their possible relations.

Similar researches have been developed in observational studies where the relations between two subsets of  $P$  are measured by their coherence. We have found that the functions used for measuring coherence are in fact functions of the dominance and separability degrees introduced in this paper. We consider that the application of dominance and separability degrees to observational studies would permit to give a detailed description of the cause-effect pattern these studies look for.

One of the uses of posets in chemistry is the ranking and prioritisation of individual objects (chemicals, regions and databases, for instance) when they have been defined by more than one of their properties. Dominance and separability degrees allow prioritising subsets of  $P$  based on the relations found in the given Hasse diagram of  $P$ . In this case we may rank complete subsets of similar chemicals, for instance, and explore their behaviour considering their order relations. Another chemical application of the concept of dominance degree was recently reported in the environmental ranking of families of refrigerants [54].

After defining and studying the mathematical properties of the dominance and separability degrees we discussed the implications that particular values  $\varepsilon = [0.5, 1)$  of dominance and  $\delta = [0.5, 1)$  of separability have over the collection of subposets of a Hasse diagram. Hence,  $<_\varepsilon$  and  $||_\delta$  were introduced as binary relations and some of their properties were studied. Special attention was dedicated to the lack of transitivity of the dominance relation  $<_\varepsilon$  and it was proved that when  $<_\varepsilon$  is equipped with a collection of  $\leq$ -paths which consider at least one element of the sequence of subposets compared, then the new relation  $(<_\varepsilon, C)$  becomes a transitive one on the collection of subsets where it is applied. This kind of transitivity dependent on the  $\leq$ -paths

between the compared subposets keeps certain resemblance with the investigations on fuzzy transitive relations developed by De Baets [55–58]. Hence the study of  $(\prec_\varepsilon, C)$  as a fuzzy transitive relation and its implications must be explored in forthcoming investigations.

From the Hasse diagram of the Born-Oppenheimer, BO, molecular total energies of the complete set of isoelectronic–isoprotonic species with total nuclear charge 10 and from its partitioning into 10 subsets containing, each one, all the objects with same number of nuclei, the following conclusions can be drawn:

1. More than half of the subsets dominate completely the others and these dominances correspond to subsets of species with more nuclei over subsets with species having fewer nuclei. This occurs because the energy of all the objects with more nuclei is greater than the energy of objects with few nuclei in more than half of the comparisons between subsets.
2. When looking for the maximum  $\varepsilon$ -value of dominance degree necessary to have a linear order showing the direct relationship between number of nuclei and BO energies it was found that it corresponds to  $\varepsilon = 0.7$ . This means that when considering all the 10 subposets, at least 70% of the pairs  $(x, y) \in P_i \times P_j$  are cases where the energy of  $x$  is higher than the one of  $y$ , with  $P_i$  gathering species with more nuclei than those collected in  $P_j$ . This result sharpens the general conclusion drawn by Daza and Bernal [32, 33] on the direct relationship between the number of nuclei and the BO energies.
3. We found that, in the majority of cases, the removing of the least energetic species of a subset  $P_i$  increases the dominance degree of  $P_i$  over other subsets. This finding suggests a systematic study of the effect of removing species on the dominance degree values. Thus, it might be analysed which objects affect in a big extent the dominance relations among groups. Studies of this sort can be regarded as the searching for “hubs” in the poset  $(\mathcal{P}, \prec_\varepsilon, C)$  and it would be interesting to find a connection between these dominance posetic hubs and the hubs studied in network theory.

When the conditions are given for having a  $\varepsilon$ -dominance Hasse diagram (Theorem 2), some of these diagrams correspond to lattices, for example those with  $\varepsilon = 0.5, 0.6$  and  $0.7$  in Fig. 6, while some other  $\varepsilon$ -values yield no lattices. It is interesting to explore the relationship between  $\varepsilon$  and the lattice character of the  $\varepsilon$ -dominance Hasse diagram.

Once calculated the dominance degrees for the subposets of a Hasse diagram, it is possible to study particular  $\varepsilon$ -values as we did in this paper when selecting  $\varepsilon = 0.5, 0.6, 0.7, 0.8$  and  $0.9$  (Fig. 6). However, is also possible, and rather interesting, to plot each  $\varepsilon$ -Hasse diagram for each dominance degree value, for example, according to Table 1 it would be worthy to select  $\varepsilon = \text{Dom}(P_j, P_i)$ , it is  $0.69, 0.73, 0.79, \dots$  to  $0.97$ . Thus, it is possible to check which pairs of subsets become incompatible when increasing  $\varepsilon$ . Although this procedure is interesting, it may be intractable because the dominance degree values might be disperse on the real interval  $(0.5, 1]$ . In such a case it is recommended clustering the dominance degree values in order to group near values in different regions of the  $(0.5, 1]$  interval. Then, the analysis of the step-by-step changes in the diagrams can be replaced by the analysis of the changes

when selecting an  $\varepsilon$ -value from each cluster. For example, if a given clustering process groups the values of  $Dom(P_j, P_i)$  (Table 1) into these four clusters: [0.9, 1], [0.81, 0.89], [0.73, 0.79], [0.69]; then it might be interesting to select a representative  $\varepsilon$ -value from each cluster and to draw the corresponding  $\varepsilon$ -dominance Hasse diagrams in order to compare them.

In spite of having found  $Dom(P_i, P_j) = 0$  and  $Dom(P_j, P_i) > Sep(P_i, P_j)$  for all the subposets considered in Fig. 5, it does not mean that this is a general result attached to the dominance and separability degrees. Those values are strictly depended on the  $\leq$ -relations among the elements in the Hasse diagram and it is usual to find values where  $Dom(P_i, P_j) > 0$  for some subposets and  $Dom(P_j, P_i) > 0$  for some others, as well as  $Sep(P_i, P_j) > 0$  for others. This diversity of dominances and separabilities makes possible to represent each ordered pair  $(P_i, P_j)$  as a point  $(Dom(P_i, P_j), Dom(P_j, P_i), Sep(P_i, P_j))$  in a Cartesian space. Following the same idea drawn before, there may be found different clusters of similar dominated and separated subposets for which is interesting to study the  $\varepsilon$ -dominance Hasse diagrams among them. An example of a Hasse diagram over which is possible to apply this procedure is the one shown in Ref. [54].

A chemical application of the measurements here developed is to the chemical elements. Klein has suggested [35] that they may be regarded as a poset and several results by Restrepo and coworkers [59–62] have shown that the groups of chemical elements correspond to similarity classes. It is worthy to calculate the dominance and separability degrees among these chemical groups in order to check the  $\varepsilon$ -dominances and  $\delta$ -separabilities among them and their possible relationship with their chemical behaviour.

In general, the dominance and separability degrees are useful mathematical tools for exploring the landscape of comparabilities and incomparabilities among subsets. Making use of them it is possible to “tune” the level of detail we want to achieve in our investigations on the order relations among subposets and this is achieved just by varying the  $\varepsilon$ - and  $\delta$ -values.

Bernal (private communication) has pointed out the resemblance of the dominance and separability formalism with that one of blockmodel used in social network analysis [63] where a graph (a poset in the current case) is given, a partition is defined and relations between elements of the partition arising from relations between elements in the parts of the partition are analysed. That set of relations between parts of the partition defines in turn a graph (a diagram in the present work) which is further analysed in order to simplify the initial graph. In short, with this procedure “one can classify the objects of the graph and, even more; one can explore the relations between classes” (Bernal, private communication).

**Acknowledgments** G. Restrepo thanks COLCIENCIAS and the Universidad de Pamplona for the grant offered during this research. G. Restrepo thanks D. J. Klein from the Texas A&M University at Galveston (USA) and A. Bernal from the Universidad Nacional de Colombia at Bogotá (Colombia) for their valuable comments and suggestions. A. Bernal is especially thanked for the detailed explanation of his work.



## References

1. R. Brüggemann, L. Carlsen, *Partial Order in Environmental Sciences and Chemistry* (Springer, Berlin, 2006)
2. I. Rival, *Algorithms and Order* (Kluwer, Dordrecht, 1989)
3. P. Annoni, Environ. doi: [10.1007/s10651-007-0041-0](https://doi.org/10.1007/s10651-007-0041-0)
4. D.L. Solomon, in *Ecological Diversity in Theory and Practice*, ed. by J.F. Grassle, G.P. Patil, W. Smith, C. Taillie (International Co-operative Publishing House, Fairland, 1979), pp. 29–35
5. E. Ruch, Theoret. Chim. Acta (Berl.) **38**, 167 (1975)
6. E. Ruch, A. Mead, Theoret. Chim. Acta (Berl.) **41**, 95 (1976)
7. E. Ruch, B. Lesche, J. Chem. Phys. **69**, 393 (1978)
8. F.A. Matsen, D.J. Klein, J. Phys. Chem. **75**, 1860 (1971)
9. E. Ruch, A. Schönhofer, Theoret. Chim. Acta (Berl.) **19**, 225 (1970)
10. E. Ruch, Accounts Chem. Res. **5**, 49 (1972)
11. I. Gutman, M. Randić, Chem. Phys. Lett. **47**, 15 (1977)
12. M. Randić, Chem. Phys. Lett. **55**, 547 (1978)
13. M. Randić, J. Math. Chem. **4**, 157 (1990)
14. M. Randić, J. Chem. Educ. **69**, 713 (1992)
15. S. El-Basil, M. Randić, Adv. Quantum Chem. **24**, 239 (1992)
16. E. Halfon, M.G. Reggiani, Environ. Sci. Technol. **20**, 1173 (1986)
17. R. Brüggemann, B. Münzer, Chemosphere **27**, 1729 (1993)
18. R. Brüggemann, B. Münzer, E. Halfon, Chemosphere **28**, 863 (1994)
19. R. Brüggemann, H.G. Bartel, J. Chem. Inf. Comput. Sci. **39**, 211 (1999)
20. S. Pudenz, R. Brüggemann, B. Luther, A. Kaune, K. Kreimes, Chemosphere **40**, 1373 (2000)
21. K. Voigt, J. Gasteiger, R. Brüggemann, J. Chem. Inf. Comput. Sci. **40**, 44 (2000)
22. R. Brüggemann, E. Halfon, G. Welzl, K. Voigt, C.E.W. Steinberg, J. Chem. Inf. Comput. Sci. **41**, 918 (2001)
23. D. Lerche, R. Brüggemann, P. Sørensen, L. Carlsen, O. J. Nielsen, J. Chem. Inf. Comput. Sci. **42**, 1086 (2002)
24. D. Lerche, P. Sørensen, R. Brüggemann, J. Chem. Inf. Comput. Sci. **43**, 1471 (2003)
25. R. Brüggemann, G. Welzl, K. Voigt, J. Chem. Inf. Comput. Sci. **43**, 1771 (2003)
26. R. Brüggemann, P.B. Sørensen, D. Lerche, L. Carlsen, J. Chem. Inf. Comput. Sci. **44**, 618 (2004)
27. R. Brüggemann, G. Restrepo, K. Voigt, J. Chem. Inf. Comput. Sci. **46**, 894 (2006)
28. G. Restrepo, R. Brüggemann, in *Recent Progress in Computational Sciences and Engineering*, ed. by T. Simos, G. Maroulis, (VSP, Leiden, 2006), pp. 1386–1389
29. G. Restrepo, R. Brüggemann, K. Voigt, Croat. Chem. Acta. **80**, 261 (2007)
30. J. Gabarro-Arpa, J. Math. Chem. **42**, 691 (2007)
31. J.R. Dias, J. Math. Chem. **4**, 17 (1990)
32. E.E. Daza, A. Bernal, J. Math. Chem. **38**, 247 (2005)
33. A. Bernal, *Ordenamientos moleculares basados en la energía* (BSc Thesis, Universidad Nacional de Colombia, Bogotá, 2004)
34. Papers in MATCH Commun. Math. Comput. Chem. **42,7** (2000); **54**, 489 (2005)
35. D.J. Klein, J. Math. Chem. **18**, 321 (1995)
36. D.J. Klein, D. Babić, J. Chem. Inf. Comput. Sci. **37**, 656 (1997)
37. I. Rival, N. Zaguia, Congressus numerantium **55**, 199 (1986)
38. G. Brightwell, P. Winkler, Order **8**, 225 (1991)
39. W.T. Trotter, *Combinatorics and Partially Ordered Sets, Dimension Theory* (The Johns Hopkins University Press, Baltimore, 1992)
40. G. Restrepo, R. Brüggemann, WSEAS Trans. Inf. Sci. Appl. **2**, 976 (2005)
41. S.T. Hedetniemi, R.C. Laskar, *Topics on Domination* (North-Holland, Amsterdam, 1991)
42. P.R. Rosenbaum, *Observational Studies* (Springer, New York, 1995)
43. P.R. Rosenbaum, Ann. Stat. **19**, 1091 (1991)
44. O. Gefeller, L. Pralle, in *Nonrandomized Comparative Clinical Studies. Proceedings of the International Conference on Nonrandomized Comparative Clinical Studies, 10–11 April 1997, Heidelberg, Germany*, ed. by U. Abel, A. Koch (Symposion Publishing, Düsseldorf, 1997).
45. P.G. Mezey, J. Am. Chem. Soc. **107**, 3100 (1985)
46. E.E. Daza, J.L. Villaveces, J. Chem. Inf. Comput. Sci. **34**, 309 (1994)

47. W. Thirring, *Acta Phys. Aust. Suppl.* **14**, 631 (1975)
48. H. Narnhofer, W. Thirring, *Acta Phys. Aust.* **41**, 281 (1975)
49. E.H. Lieb, B. Simon, *J. Phys. B.* **11**, 1537 (1978)
50. P.G. Mezey, *Theor. Chim. Acta.* **59**, 321 (1981)
51. P.G. Mezey, *Int. J. Quant. Chem.* **22**, 101 (1982)
52. P.G. Mezey, *Mol. Phys.* **47**, 121 (1982)
53. P.G. Mezey, *J. Chem. Phys.* **80**, 5055 (1984)
54. G. Restrepo, W. Weckert, R. Brüggemann, S. Gerstmann and H. Frank, submitted to *Environ. Sci. Technol.*
55. B. De Baets, H. De Meyer, *Soft Comput.* **7**, 210 (2003)
56. B. De Baets, H. De Meyer, *Inform. Sci.* **152**, 167 (2003)
57. H. De Meyer, H. Naessens, B. De Baets, *Eur. J. Oper. Res.* **155**, 226 (2004)
58. B. De Baets, H. De Meyer, B. De Schuymer, S. Jenei, *Soc. Choice Welfare* **26**, 217 (2006)
59. G. Restrepo, H. Mesa, E. Llanos, J.L. Villaveces, *J. Chem. Inf. Comput. Sci.* **44**, 68 (2004)
60. G. Restrepo, J.L. Villaveces, *Croat. Chem. Acta* **78**, 275 (2005)
61. G. Restrepo, E.J. Llanos, H. Mesa, *J. Math. Chem.* **39**, 401 (2006)
62. G. Restrepo, H. Mesa, E. Llanos, J.L. Villaveces, in *The Mathematics of the Periodic Table*, ed. by R.B. King, D.H. Rouvray (Nova, New York, 2006), pp. 75–100
63. W. de Nooy, A. Mrvar, V. Batagelj, *Exploratory Social Network Analysis with Pajek* (Cambridge University Press, Cambridge, 2006)