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Prolegomenon on Partial Orderings in Chemistry

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Motivational Overture

Partial orderings allow a general way of making comparisons, such as in chemistry are so often of central relevance. Now and again in chemistry (and elsewhere) there is encountered a characteristic to which various investigators ascribe different numerical values for the same molecule independently of any perceived imprecision in experiment. As examples (in chemistry) one might mention "electronegativity", or "aromaticity", or "reactivity", or degree of "branching", or degree of "chirality". Often the ambiguity is imagined to be due to some conceptual "short-coming" which if only rectified by a correct numerically valued definition (as advocated by one author or another), then there would result "true" or "correct" values for the particular characteristic. But there is another possibility - namely that such characteristics are non-numerical quantities. Perhaps many of these characteristics do not lead to a total ordering of the objects (e.g., molecules or even certain properties thereof) being so characterized. That is, the various ascriptions of numerical values by different investigators would be just different partly faithful representations of an underlying "partial ordering". Perhaps then the idea of "partial ordering" is a fundamental and hopefully useful concept cosmopolitanly implicit throughout much of chemistry - and presumably too it is of relevance throughout many other scientific fields, allowing one to make comparisons in a rather general way.

Thence the general idea of "partial orderings" is to be considered in this special issue of MatCh. General features are to be developed and particular chemical examples are to be explored, ranging somewhat beyond even the examples already alluded to. Indeed such partial-ordering chemical ideas are found implicitly in the works of a number of authors usually in the context of a special application, e.g., for degrees of molecular "branching", for degrees of "chirality", or for molecular "similarity", or for molecular "shape", or for "acidity", or for "aromaticity", or for chemical "periodicity".

Fundaments & General History of Partial Orderings

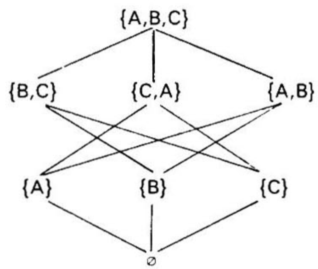
Beyond the bounds of chemistry the idea of partial orderings has wide application - the abstract idea presumably being traceable in some form back to W. Leibniz, as noted in Garrett Birkhoff's seminal book [1] giving much prominence to the mathematics of posets (and refinements therebeyond). Birkhoff notes "The world around us abounds with examples of partly ordered sets", and there are many texts attesting to this, at least in-so-far as the mathematical world is concerned. Formally one defines a *partial ordering* on a set $\mathcal{P}$ as a binary relation $\leq$ satisfying so-called "reflexivity", "antisymmetry", & "transitivity" conditions

$$A \in \mathcal{P} \;\Rightarrow\; A \leq A$$

$$A \leq B \;\&\; B \leq A\;,\; A,B \in \mathcal{P} \;\Rightarrow\; A = B$$

$$A \leq B \;\&\; B \leq C\;,\; A,B,C \in \mathcal{P} \;\Rightarrow\; A \leq C$$

and the set $\mathcal{P}$ along with its partial ordering is referred to as a partially ordered set, or more briefly as a *poset*. Birkhoff tends to give rather "mathematical" examples such as: the subset partial ordering of the family of subsets of a parent set; or the divisor partial ordering of the set of positive integers. A less formally mathematical example is that involving a collection of shapes cut from paper, and $A \leq B$ is to mean that "shape A placed flat on a table top can be completely covered by shape B". Another example is of a genealogical tree where $A \leq B$ is identified to mean "A is a descendant of B". Often such a genealogical tree is presented graphically with lines from each member to its direct off-spring drawn in such a way that descendants lie "lower" in the diagram. Such a presentation termed a *Hasse diagram* applies for rather general posets. *E.g.*, for the subset partial ordering of a parent set {A,B,C} the Hasse diagram is



(where ∅ denotes the empty set).

In the definition of a poset the "antisymmetry" condition may be relaxed so that $A \leq B$ & $B \leq A$ implies "equivalence" of A & B rather than identity of A & B, in which case the relation $\leq$ is called a *quasi-order.* Still one can think of a partial ordering, now on the set of equivalence classes. In any event partial orders clearly entail a less stringent constraint than that of total order (where also $A,B \in \mathcal{P}$ would imply $A \leq B$ or $B \leq A$).

Frequently functions from a poset $\mathcal{P}$ to the real numbers $\mathcal{R}$ are of relevance. Of special interest is a type of function f that preserves the ordering from $\mathcal{P}$ onto the reals, in the sense that

$$A \leq B \text{ in } \mathcal{P} \quad \Rightarrow \quad f(A) \leq f(B) \text{ in } \mathcal{R}$$

Such functions have been given many names, including "Schur convex", or "partial-ordering homomorphic" or "order-preserving" or "isotonic". Regardless of the name it is these functions that may be viewed as partly faithful numerical representations of an underlying partial ordering.

As a mathematical program Gian-Carlo Rota constructively proposed [2] that partial orderings are foundational for the whole field of combinatorics. A proto-typical occurrence involves a sum of the form

$$X(a) = \sum_{b \in \mathcal{P}} f(a,b) x(b)$$

with the "cluster function" f satisfying

$$f(a,b) = 0 \quad , a \neq b \leq a$$

A special case of frequent interest is the so-called "zeta" function with all the non-zero values being 1. Also often one may append an extra (diagonal) condition that $f(a,a) \neq 0$, whence the f(a,b) are "invertable", so that the x(a) can be expressed in terms of the X(b). Indeed in combinatorics X(a) & x(a) often represent two different types of (evidently inter-related) enumerations, and the inversion to obtain x in terms of X is of significance. E.g., for the subset partial ordering, such ideas yield directly the so-called "principle of exclusion/inclusion". Generally a powerful "incidence" algebra (involving a matrix-multiplication-like convolution product on cluster functions) ensues, and in combinatorics texts of the last few decades the central role for Rota's posetic ideas seems to have become accepted.

There is much other mathematics involving posets. Birkhoff's book [1] ends up focusing on a special interesting type of "bidirectionally ordered" poset known as a "lattice". (Basically a lattice is a poset for which every pair of elements has a unique "least upper bound" & a unique "greatest lower bound".) Also there are several more recent mathematics books [3,4,5] focusing on partial orderings. A collection of mathematical overviews of posets with emphasis on different applications (other than in chemistry & physics) is available [6]. In biology & ecology one may view evolutionary fittness, evolutionary (or phylogenetic) trees, &

food-webs each as providing examples of partial orderings. And one may imagine that many common-place aspects of our every-day world might be partially ordered - things such as "intelligence" and "quality of life", or also "truth" and "beauty". But next a consideration may be made of the history of chemical research in which there has been advocated a significant role for posets.

Posets in Chemistry

Especially notably, partial orderings have been persistently studied by Ernst Ruch & co-workers [8], who have focused on developing a poset involving a complementary pair of aspects: of "identification/distinction", or of "order/disorder", or of "symmetry/antisymmetry", or (in terms of Young diagrams) of "row/column"). This underlying Young-diagram (or "majorization") poset is presented in this work to be of fundamental importance, as also is attested to by its appearance [5] in a wide range of applications in economics, statistics, & mathematics. Ruch & co-workers have focused on "mixedness" and related generalized distance functions on this partial ordering. For chemistry there are particular results, as for a broad class of irreversible many-body processes, a strengthened version of the second law of thermodynamics with time & entropy being identified as but two isotonic functions on this partial ordering. Moreover, at Ruch's apparent instigation, several researchers (I. Gutman, M. Randić, & W. Hässelbarth) [8] have made an interesting application characterizing the "degree of branching" of a molecular graph. There are a number of independent considerations of this poset in a chemico-physical realm [9], and Ruch's ideas have motivated yet further articles [10]. Recently the same Young-diagram poset lattice emerges in the culmination [11] of some decades of mathematical work relating a general matrix's "Segre characteristic" (characterizing the eigen-spectrum) and what might be termed the "Frobenius characteristic" (characterizing the permutation-blockable form of the matrix).

From a somewhat different point of view there are posetic chemical applications involving a general property represented as vectorial collections of scalar properties. Milan Randić & C. Wilkins [12] have focused on the use of such partial orderings to elucidate graph-theoretic aspects of molecular structure. With values for two simple graph-theoretic invariants plotted along x- & y-coordinates these workers obtain an array of points each characterizing a molecule and such that when the plot is oriented properly the points corresponding to molecules lower on the diagram are identified as lesser in a partial ordering (or quasi-ordering), associated to the orderings of several physical properties. In application to alkanes (using the number of length-2 paths & of length-3 paths as the two graph invariants) the resulting Hasse diagram is termed a "periodic chart of alkane isomers". Ivan Gutman & F. Zhang along with co-workers also utilize [13] chemical graph-theoretic indices to introduce (presumably chemically meaningful) partial orderings, associated to π-energies of acyclic conjugated hydrocarbons. There are other related chemical ideas [14].

Significantly Halflon, Brüggemann, & co-workers [15] have developed a poset-centered scheme to organize various possible environmental pollutants, and thereby they find aid in hazard assessment. There have been a number of applications, including also some to structure/property correlations. Recently such ideas are variously presented by several groups in the proceedings [16] of a workshop on "Order Theoretical Tools in Environmental Sciences". In a related sort of development Bartel [17] has developed a posetic scheme of "concept analysis".

Another general chemical application concerns the construction of chemical sub-structural cluster expansions, where the relevant poset is that of the substructures of a parent structure, and some use of Rota's Möbius-algebraic ideas have been considered [18]. These applications are in close concert with many earlier empirical expansions of molecular properties in terms of molecular sub-structures, e.g., heats of formation expressed in terms of bond energies (and at the next higher order one includes 3-site terms for neighboring bonds, though there are even higher-order terms corresponding to larger sub-structures). But despite the long-standing chemical interest in such sub-structural characterization (perhaps described as "additivity" or "group-additivity" or "group-function" schemes), only occasionally has there been explicit reference to the formal theory of partial orderings. In the general theory the molecular property so expanded need not be "additivite", such general properties including model Hamiltonians or molecular wave-functions. Related ideas (dating back to Mayer & Uhlenbeck in the 1930s) have been developed in a many-body statistical mechanical framework, and there are results presented [19] in an elegant graph-theoretico-posetic framework. Also there are a number of more chemically oriented works [20] in this area.

A related sort of partial ordering concerns the combinatorial aspects of the vertices, edges, faces, & cells of various topological "complexes" relevant in describing molecular geometric structures. The partial ordering is that of being "contained in (the boundary)", and Möbius inversion leads to the fundamental topo-combinatorial Euler (or Euler-Poincare) relation. *E.g.*, as applied to polyhedra this Euler relation implies that every "fullerene" (with all faces of 5 or 6 sides) has exactly 12 pentagons. The posetic nature & relevant Möbius algebra is recognized in mathematics but is rather infrequently described in such a fashion in chemistry - though see [21].

Yet a further occurrence of posets in chemistry arises in considering the set of subgroups of a parent group. This poset in fact forms a "lattice", and is of relevance in tracing patterns of "descent in symmetry", *e.g.*, as applied in ligand-field-theoretic contexts [22], using ideas involving "iso-scalar factors", "fractional parentage coefficients", & "recoupling coefficients", with typically little reference to the combinatorial theory of posets, but with a rich physics-oriented literature [23] ultimately dating back to Racah, Wigner, & Jahn. Often emphasis is on sequences of subgroups (which then is totally ordered), but then there are recoupling coefficients from one chain to another (whence a non-trivial partial ordering is at least implicit). Another application of the subgroup poset involves Pólya-theoretic enumeration [24] of molecular substitutional patterns of different subsymmetries of a fixed skeletal symmetry. Notably central in this application is a Möbius function which is the inverse to a zeta function (described as a "table of Marks"), and the ideas also overlap with work of Ruch & others [6-10].

In a broad chemical context partial orderings have been argued [25] to be of fundamental relevance for many chemical concepts (such as acidity, or aromaticity, or reactivity, or molecular toxicity, or molecular shape, or molecular symmetry, or molecular similarity), where there is more than one reasonable definition or way to measure a property. That is, multi-dimensional aspects of a property are argued to be naught but the manifestation of the occurrence of a non-trivial (*i.e.*, non-totally ordered) poset, and some mathematical tools are developed in a chemical context to deal with such posetic multi-dimensionality. There is overlap with communications from Prof. Ruch and with the earlier work of Randić, Gutman, & others [12,13,14], as well as with the extensive environmental-science-oriented work of Brüggemann & others [15,16] and with Bartel's [17] chemometric-oriented scheme, where (in all these cases) posets play a central role.

There are numerous cases in chemical research where it appears that posets are implicit. A number of such cases are briefly indicated in [25]. One frequent sort of circumstance susceptible to a posetic interpretation involves that where there are levels of refinement of description, e.g., as involves different types of isomers (permutational, structural, valence, geometric, stereo, "bond-stretch", "isotopic", *etc.*). That is, one may view different isomer classifications as grouping different conformations together in different sorts of isomer sets, and then invoke the subset partial ordering. Or in order to affect the isomer classifications one may implement a decision tree (*e.g.*, [26]) which clearly is a poset, though often not explicitly recognized as such. Subset & subgraph ordering relations are not total orderings, but are so very frequently encountered that a referencing of these occurrences which do not explicitly utilize combinatorial (*e.g.*, Möbius-algebraic) posetic methodology has not been attempted. In fact there are likely numerous applications of the Möbius inversion perhaps under the description of the "principle of inclusion & exclusion", and these applications we have not noted. Another chemical occurrence involves (directed) reaction diagrams, as discussed in an article in the present issue of MatCh. One may surmise that making explicit the occurrence of posets in variety of different contexts could often substantively aid in formulating & dealing with associated applications.

In physics there are some further diverse applications of presumable relevance for chemistry, and a few such are indicated in [27]. In mathematics there again are numerous papers, with references indicated in [3,4,5], and further references for applications in several other sciences are indicated in [5,6].

Thence it seems that there is a wide-ranging diversity of possible applications of partial orderings in chemistry, and other areas. Perhaps posets provide a case of Coulson's [28] "primitive pattern of understanding". This special issue of MatCh is to encourage the development of this promising theoretical structure, with several chemically relevant articles now following.

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