Journal of Mathematical Chemistry 16 (1994) 245–256

Chemical algebra. I: Fuzzy subgroups

Remi Chauvin

Laboratoire de Chimie de Coordination du C.N.R.S., Unité 8241, liée par convention à l'Université Paul Sabatier, 205 Route de Narbonne, 31 077 Toulouse Cedex, France

Received 7 July 1994

Using the notion of fuzzy subset, the algebraic formulation of the constant of stereogenic pairing equilibria between skeletal analogs (previously disclosed) is connected to symmetry group theory. A distinction is introduced between geometrical (skeletal) symmetry and topographical (numerical parameters) symmetry. In order to describe "topographical symmetry", a formal extended definition of a subgroup is proposed. Fuzzy subsets of the skeletal group G are endowded with a structure which can be defined without referring to the geometrical representation of the abstract group isomorphic to G. The relevance of these propositions is evidenced by their "integer interpretation" meeting basic definitions of group theory, as well as by their role in expressing chemical pairing constants.

1. Introduction

The starting point is the shift of the pairing equilibrium

$$2\mathbf{u}_1/\mathbf{u}_2 \rightleftarrows \mathbf{u}_1/\mathbf{u}_1 + \mathbf{u}_2/\mathbf{u}_2\,,$$

where $\mathbf{u}_1$ and $\mathbf{u}_2$ represent two molecules interacting with each other or with themselves. The equilibrium constant (or "pairing product") is

$$K = \frac{[\mathbf{u}_1/\mathbf{u}_1][\mathbf{u}_2/\mathbf{u}_2]}{[\mathbf{u}_1/\mathbf{u}_2]^2}\,,$$

where $[\mathbf{u}_i/\mathbf{u}_j]$ denotes the concentration of the paired species $\mathbf{u}_i/\mathbf{u}_j$.

As an example, metathesis of olefins can be regarded as a stereogenic pairing equilibrium where the stereogenicity corresponds to the cis/trans isomerism, and where the symmetrized skeleton corresponds to an idealized geometry (e.g. the geometry of the symmetric carbene H_2C:) (see fig. 1).

A general algebraic formulation has been proposed and discussed on the basis of three hypothesis [1,2].

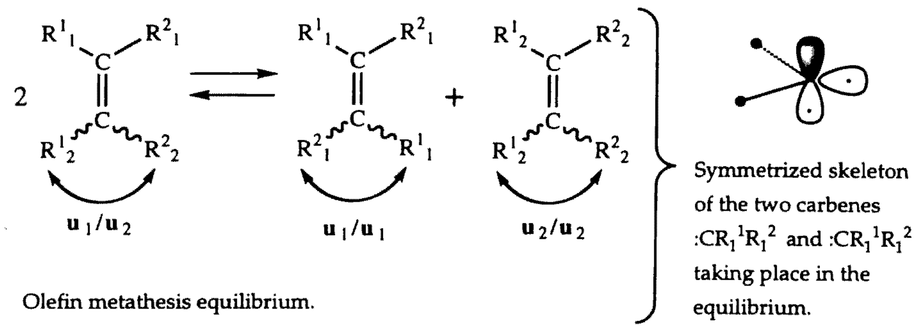

Fig. 1.

(1) *Skeleton symmetrization*: skeletons of interacting molecules are identically symmetrized in a realistic manner.

(2) *Skeleton overlap pairing*: the geometry of the paired species is the juxtaposition of the two skeletons, in such a manner that they are parallel and close to each other.

(3) *Scalar product form of the ligand interactions*: only one kind of pairwise ligand interaction occurs, and the corresponding energy is proportional to a scalar product between real or vector ligand parameters assigned to skeletal sites.

Considering the pairing stereogenicity resulting from the symmetry of the skeleton as an "entropic contribution", the pairing equilibrium constant has been expressed by

$$K = \frac{\left(\sum_g \exp\left[-\frac{a(g\mathbf{u}_1|\mathbf{u}_1)}{r^q kT}\right]\right)\left(\sum_g \exp\left[-\frac{a(g\mathbf{u}_2|\mathbf{u}_2)}{r^q kT}\right]\right)}{\left(\sum_g \exp\left[-\frac{a(g\mathbf{u}_1|\mathbf{u}_2)}{r^q kT}\right]\right)^2},$$

where $a(g\mathbf{u}_i|\mathbf{u}_j)/r^q$ is the interaction energy in the pair $g\mathbf{u}_i/\mathbf{u}_j$: a and q are fixed parameters with $a<0$, r is the (short) distance between the paired species.

Many recent efforts focus on the quantification of molecular similarity [3]. In this prospect, conditions are sought to make K reflect "how much skeletal analogs $\mathbf{u}_1$ and $\mathbf{u}_2$ have similar topographies". The consistency of such a quantification by $1/K$ requisitions the following conditions:

(a) $0 \leqslant 1/K \leqslant 1$.

(b) $1/K = 1 \Rightarrow \mathbf{u}_1$ and $\mathbf{u}_2$ are chemically equivalent: $\mathbf{u}_1 = g_0\mathbf{u}_2$ for some skeletal symmetry operation g_0 (the converse implication is always satisfied).

For C_1 (or C_i or C_s) and for C_2 (or C_{2h} or C_{2v} or S_4) skeletal symmetries, these properties have been proved regardless of the nature (real number or vector) and the values of the ligand parameters. They have been discussed for carbene dimerization equilibria, equilibrating Diels-Alder reactions and equilibrating cyclopropanation reactions, where the pairing stereogenicity corresponds to a cis/trans isomerism [1].

The model has been also applied to chemical chirality in order to answer the following question: if $\mathbf{u}$ and $\mathbf{v}$ are isomers which do not interconvert by any rotation but which interconvert by an improper isometry σ (mirror, inversion, reflection-rotation: $\mathbf{v} = \sigma\mathbf{u}$), is the homochiral association (RR) or (SS) more stable than the heterochiral one (RS)? In this context, properties (a) and (b) have been proved to be fulfilled by $K(\mathbf{u}, \sigma\mathbf{u})$ for several skeletal symmetries whatever the molecular vector $\mathbf{u}$ is [2].

The scalar product form of the interaction energy entails the following expression:

$$K = \frac{\left(\sum_g \exp\left[\frac{a}{2r^q kT}\|g\mathbf{u}_1 - \mathbf{u}_1\|^2\right]\right)\left(\sum_g \exp\left[\frac{a}{2r^q kT}\|g\mathbf{u}_2 - \mathbf{u}_2\|^2\right]\right)}{\left(\sum_g \exp\left[\frac{a}{2r^q kT}\|g\mathbf{u}_1 - \mathbf{u}_2\|^2\right]\right)^2}.$$

The quantities $\mu_{ij}(g) = \exp[-\|g\mathbf{u}_i - \mathbf{u}_j\|/\sqrt{2}]$ lie between 0 and 1, and consistently quantify "how much the skeletal symmetry operation g makes $\mathbf{u}_i$ coincide with $\mathbf{u}_j$": replacing $1/K$ by $\mu_{ij}(g)$ (for each operation g) in the requirements (a) and (b), the analogous requirements for $\mu_{ij}(g)$ are easily verified.

Description of symmetry comes under group theory [4]. In this realization, abstract groups G act by permuting points (when the number of mathematical entities is finite or countable, the action is called a permutation representation of G). Descent of symmetry from a highly symmetric structure to a lower one is termed as a group–subgroup relationship: when the structure is constituted by skeletal sites in a molecule, this relationship is represented by a group lattice [2,5]. For $i = j$, the set of the values $\mu_{ii}(g)$ characterizes the "symmetry of the molecular topography" of $\mathbf{u}_i$ (the term "topography" refers to the information corresponding to the assignment of atoms on a skeleton already bearing the informations of "topology" and "geometry"). Indeed, the exact symmetry of $\mathbf{u}$ is characterized by those operations g for which $\mu_{ii}(g) = 1$: they constitute a subgroup of the skeletal symmetry group G.

Quite generally, a system can be described in a two-step process. At the outset, a basic model (a general equation, a molecular skeleton, etc.) is selected, which is characterized by some symmetry. When this model is applied to a particular system, some symmetries are lost as a result of either geometrical boundaries or topographical boundaries (disymmetry in the assignment of local parameters). Arbitrary geometrical skeletons are currently drawn to account for site-permutational effects of the molecular point-group. However, the actual space-arrangements of ligands can be "more symmetrical" than these graphical representations, where the space non-equivalence of sites is exaggerated. In order to take advantage of such geometrical approximations, symmetrized skeletons are considered.

On the other hand, the symmetry of the topography of the molecule also depends on some approximations (e.g. a hydrogen atom and a deuterium atom will be considered chemically equivalent provided that isotopic effects can be neglected). Perturbational methods rely on such approximations. Unlike geometry, topography is not completely described by group theory. In order to introduce a mathematical definition of pairing product, we seek means to describe "topographical symmetries" as intermediates in a lattice of symmetry groups. Referring to Zadeh's definition of fuzzy subsets, the functions $\mu_{ii}(g)$ defined above are suitable for this goal [6].

However, these functions are defined with respect to the chemical representation of the skeletal group G. We aim at defining more general membership functions μ by only some of the properties induced by the norm taking place in the expression of $\mu_{ii}(g)$: the fuzzy subsets defined like this would have a structure which is independent of the group representation considered, like the structure of abstract groups does not depend on the geometrical realization. Whereas the concept of fuzzy set (fuzzy logic) has been already introduced in conformational analysis [7], analytical chemistry [8] and epistomological definition of chirality [9], it is here used in symmetry theory.

2. Basic propositions

Given a set S, a subset A of S is completely defined by its characteristic (or membership) function μ_A on S: $\forall s \in S, \mu_A(s) = 1$ if $s \in A$, and $\mu_A(s) = 0$ otherwise. In a generalization process, a "fuzzy subset of S" is defined by a real valued map $\mu_{\underline{A}}$, such that: $\forall s \in S, 0 \leqslant \mu_{\underline{A}}(s) \leqslant 1$: $\mu_{\underline{A}}(s)$ specifies the membership level of all elements of S to some criterion "$\underline{A}$" [6].

DEFINITION 1

Let G be a group. A fuzzy subset $\underline{A}$ of G is called a "fuzzy subgroup of G" if its membership function $\mu_{\underline{A}}: G \rightarrow [0, 1]$ fulfills the requirements

(i) $\underline{A}$ contains a trivial element, i.e. $\exists g \in G, \mu_{\underline{A}}(g) = 1$.
(ii) $\forall (g, h) \in G^2, \mu_{\underline{A}}(g) \cdot \mu_{\underline{A}}(h) \leqslant \mu_{\underline{A}}(gh)$.
(iii) $\forall g \in G, \mu_{\underline{A}}(g) = \mu_{\underline{A}}(g^{-1})$.

The neutral element of G, e, is a trivial element of any fuzzy subgroup $\underline{A}$ of G (if $\mu_{\underline{A}}(g) = 1$, taking $h = g^{-1}$ in the condition (ii), we get from (iii): $1 \times 1 \leqslant \mu_{\underline{A}}(gh) = \mu_{\underline{A}}(e) \leqslant 1 \Rightarrow \mu_{\underline{A}}(e) = 1$).

Since it is obvious that a trivial subgroup of G is a fuzzy subgroup of G, this definition is an extension of the definition of a subgroup of G.

The "trivial part" of $\underline{A}$ defined as $T(\underline{A}) = \{g \in G, \mu_{\underline{A}}(g) = 1\}$, is a trivial subgroup. $B(\underline{A}) = \{g \in G, \mu_{\underline{A}}(g) \neq 0\}$, is also a trivial subgroup of G: by restriction of G to $B(\underline{A})$, only subgroups $\underline{A}$ which fulfill the condition: $\forall g \in G, \mu_{\underline{A}}(g) \neq 0$, are considered.

PROPOSITION 1

If $\underline{A}$ is a fuzzy subgroup of G, then: $\underline{A} = G \Leftrightarrow \forall (g,h) \in G^2, \mu_{\underline{A}}(g)\mu_{\underline{A}}(h) = \mu_{\underline{A}}(gh)$.

Proof

$\Rightarrow$ is obvious

For $\Leftarrow$, let g belong to G. Taking $h = g^{-1}$, we get: $\mu_{\underline{A}}(g) \cdot \mu_{\underline{A}}(g^{-1}) = \mu_{\underline{A}}(e) = 1$. Thus, according to (iii): $[\mu_{\underline{A}}(g)]^2 = 1$, and: $\forall g \in G, \mu_{\underline{A}}(g) = 1$, i.e. $\underline{A} = G$. □

PROPOSITION 2

Suppose that h is any trivial element of $\underline{A}(\mu_{\underline{A}}(h) = 1)$. Then

$$\forall g \in G, \mu_{\underline{A}}(gh) = \mu_{\underline{A}}(hg) = \mu_{\underline{A}}(g).$$

Proof

The requirement (ii) affords both the following inequalities:

$$\mu_{\underline{A}}(g)\mu_{\underline{A}}(h) \leqslant \mu_{\underline{A}}(gh) \quad \text{and} \quad \mu_{\underline{A}}(gh)\mu_{\underline{A}}(h^{-1}) \leqslant \mu_{\underline{A}}(ghh^{-1}) = \mu_{\underline{A}}(g).$$

Since $1 = \mu_{\underline{A}}(h) = \mu_{\underline{A}}(h^{-1})$ (from (iii)): $\mu_{\underline{A}}(g) = \mu_{\underline{A}}(gh)$. Likewise, the equality $\mu_{\underline{A}}(g) = \mu_{\underline{A}}(hg)$ is easily obtained. □

REMINDER

A fuzzy subset $\underline{A}$ of G is said to be "included" in another one $\underline{B}$, if

$$\forall g \in G, \quad \mu_{\underline{A}}(g) \leqslant \mu_{\underline{B}}(g).$$

The intersection of two fuzzy subsets $\underline{A}$ and $\underline{B}$ can be defined either by:

$$\mu_{\underline{A} \cap \underline{B}}(g) = \mu_{\underline{A}}(g) \cdot \mu_{\underline{B}}(g) \tag{1}$$

or by

$$\mu_{\underline{A} \cap \underline{B}}(g) = \text{Min}[\mu_{\underline{A}}(g); \mu_{\underline{B}}(g)]. \tag{2}$$

PROPOSITION 3

Whatever is the definition (1) or (2) of the intersection of two fuzzy subsets, the intersection of two fuzzy subgroups of G is a fuzzy subgroup of G.

Proof

- The result is obvious for definition (1).
- If the definition (2) is retained:

(i) $\mu_{\underline{A}\cap\underline{B}}(e) = \text{Min}[\mu_{\underline{A}}(e); \mu_{\underline{B}}(e)] = \text{Min}[1; 1] = 1$, and e is a trivial element of $\underline{A} \cap \underline{B}$.

(ii) $\forall (g, h) \in G^2$, $\mu_{\underline{A}\cap\underline{B}}(gh) = \text{Min}[\mu_{\underline{A}}(gh); \mu_{\underline{B}}(gh)]) \geqslant \text{Min}[\mu_{\underline{A}}(g)\mu_{\underline{A}}(h); \mu_{\underline{B}}(g)\mu_{\underline{B}}(h)]$

$$\geqslant \text{Min}[\mu_{\underline{A}}(g); \mu_{\underline{B}}(g)] \cdot \text{Min}[\mu_{\underline{A}}(h); \mu_{\underline{B}}(h)] = \mu_{\underline{A}\cap\underline{B}}(g)\mu_{\underline{A}\cap\underline{B}}(h).$$

(iii) $\forall g \in G$, $\mu_{\underline{A}\cap\underline{B}}(g^{-1}) = \text{Min}[\mu_{\underline{A}}(g^{-1}); \mu_{\underline{B}}(g^{-1})] = \text{Min}[\mu_{\underline{A}}(g); \mu_{\underline{B}}(g)] = \mu_{\underline{A}\cap\underline{B}}(g)$.

3. Cosets of a group G by its fuzzy subgroups

DEFINITION 2

Let G be a group, and $\underline{A}$ be a fuzzy subgroup of G. For any element g in G, the "fuzzy right class (resp. left class) of g modulo $\underline{A}$", is the fuzzy subset of G, $g\underline{A}$ (resp. $\underline{A}g$), defined with the membership function:

$$\forall h \in G, \quad \mu_{g\underline{A}}(h) = \mu_{\underline{A}}(g^{-1}h) \quad (\text{resp. } \mu_{\underline{A}g}(h) = \mu_{\underline{A}}(hg^{-1}))\,.$$

The (trivial) set of the fuzzy right (resp. left) classes modulo $\underline{A}$ is called "right (resp. left) coset of G by $\underline{A}$", and is denoted $G/\underline{A}$ (resp. $\underline{A}\backslash G$).

DEFINITION 3

Let $\underline{E}$ and $\underline{F}$ be two fuzzy subsets of a group G. The "product of $\underline{E}$ by $\underline{F}$" is defined as the fuzzy subset $\underline{E} \bullet \underline{F}$ with the membership function:

$$\forall h \in G, \quad \mu_{\underline{E}\bullet\underline{F}}(h) = \underset{g\in G}{\text{Max}}[\mu_{\underline{E}}(g) \cdot \mu_{\underline{F}}(g^{-1}h)]\,.$$

PROPOSITION 4

The set of all the fuzzy subsets of a finite group G endowed with the product "$\bullet$" is a monoid. It is denoted by $\underline{P}(G)$.

Proof

By construction, the operation "$\bullet$" is internal in $\underline{P}(G)$. Let us show that it is associative. Let $\underline{D}$, $\underline{E}$ and $\underline{F}$ be three fuzzy subsets of a finite group G.

$$\begin{aligned}\forall s \in G, \quad \mu_{(\underline{D}\bullet\underline{E})\bullet\underline{F}}(s) &= \underset{g\in G}{\text{Max}}[\mu_{\underline{D}\bullet\underline{E}}(g) \cdot \mu_{\underline{F}}(g^{-1}s)] \\ &= \underset{g\in G}{\text{Max}}\left\{\left[\underset{h\in G}{\text{Max}}[\mu_{\underline{D}}(h)\mu_{\underline{E}}(h^{-1}g)]\mu_{\underline{F}}(g^{-1}s)\right]\right\} \\ &= \underset{g,h\in G}{\text{Max}}[\mu_{\underline{D}}(h) \cdot \mu_{\underline{E}}(h^{-1}g) \cdot \mu_{\underline{F}}(g^{-1}s)] \\ &= \underset{g',h\in G}{\text{Max}}[\mu_{\underline{D}}(h) \cdot \mu_{\underline{E}}(g') \cdot \mu_{\underline{F}}(g'^{-1}h^{-1}s)] \quad (\text{where } g = hg') \\ &= \mu_{\underline{D}\bullet(\underline{E}\bullet\underline{F})}(s)\,.\end{aligned}$$

Following the same process as in group theory, we seek a condition on $\underline{A}$ ensuring that the subset $G/\underline{A}$ of $\underline{P}(G)$ has a group structure for the product "•". Let $\underline{A}$ be a fuzzy subgroup of G. If $\underline{E}$ and $\underline{F}$ are two right classes $h\underline{A}$ and $k\underline{A}$ modulo $\underline{A}$, their product is given by

$$\forall s \in G, \mu_{h\underline{A} \bullet k\underline{A}}(s) = \operatorname*{Max}_{g \in G}[\mu_{\underline{A}}(h^{-1}g) \cdot \mu_{\underline{A}}(k^{-1}g^{-1}s)]\,. \qquad \square$$

DEFINITION 4

A fuzzy subgroup $\underline{A}$ of G is said to be "normal in G" if its membership function is central on G, i.e. if: $\forall (g,h) \in G^2, \mu_{\underline{A}}(hgh^{-1}) = \mu_{\underline{A}}(g)$.

This provides an extension of the definition of normal (trivial) subgroups of G.

THEOREM 1

If $\underline{A}$ is a fuzzy subgroup of G, then $(G/\underline{A}, \bullet)$ is a group if and only if $\underline{A}$ is normal in G. Moreover: $\forall (g\underline{A}, h\underline{A}) \in (G/\underline{A})^2, g\underline{A} \bullet h\underline{A} = (gh)\underline{A}$ and $(G/\underline{A}, \bullet)$ is isomorphic to $G/T(\underline{A})$.

Proof

(a) $G/\underline{A}$ contains $\underline{A} = e\underline{A}$.

(b) The operation "•" is internal in $G/\underline{A}$: $\forall (h,k,s) \in G^3$,

$$\begin{aligned}\mu_{\underline{A}}(h^{-1}g) \cdot \mu_{\underline{A}}(k^{-1}g^{-1}s) &= \mu_{\underline{A}}(h^{-1}g) \cdot \mu_{\underline{A}}(g^{-1}sk^{-1}) \quad (\underline{A} \text{ is normal in } G)\\ &\leqslant \mu_{\underline{A}}(h^{-1}gg^{-1}sk^{-1}) = \mu_{\underline{A}}(h^{-1}sk^{-1}) \quad (\underline{A} \text{ is a fuzzy subgroup})\\ &\leqslant \mu_{\underline{A}}(k^{-1}h^{-1}s) = \mu_{(hk)\underline{A}}(s) \quad (A \text{ is normal in } G)\end{aligned}$$

Therefore,

$$\mu_{h\underline{A} \bullet k\underline{A}}(s) = \operatorname*{Max}_{g \in G}[\mu_{\underline{A}}(h^{-1}g)\mu_{\underline{A}}(k^{-1}g^{-1}s)] \leqslant \mu_{(hk)\underline{A}}(s) = \mu_{\underline{A}}(k^{-1}h^{-1}s)\,.$$

For $g = h, \mu_{\underline{A}}(h^{-1}g) \cdot \mu_{\underline{A}}(k^{-1}g^{-1}s)$ matches the right term and, hence, the Max value. Consequently, $\mu_{h\underline{A} \bullet k\underline{A}}(s) = \mu_{(hk)\underline{A}}(s)$, and $h\underline{A} \bullet k\underline{A} = (hk)\underline{A} \in G/\underline{A}$.

(c) The operation is associative (proposition 4).

(d) $e\underline{A} = \underline{A}$ is the neutral element of $G/\underline{A}$.

(e) From (b), the inverse element of $g\underline{A}$ is $g^{-1}\underline{A}$.

(f) $\forall (g,h) \in G^2, h \in T(g\underline{A}) \Leftrightarrow \mu_{\underline{A}}(g^{-1}h) = 1 \Leftrightarrow g^{-1}h \in T(\underline{A}) \Leftrightarrow h \in gT(\underline{A})$.

Thus, $\forall g \in G, T(g\underline{A}) = gT(\underline{A})$. This allows the biunivocal function τ: $G/\underline{A} \rightarrow G/T(\underline{A})$, to be defined by: $\forall g \in G, \tau(g\underline{A}) = gT(\underline{A})$.

Since $\underline{A}$ is a normal fuzzy subgroup of G, $T(\underline{A})$ is a normal subgroup of G. Indeed,

$\forall g \in G, \forall h \in T(\underline{A}), \mu_{\underline{A}}(ghg^{-1}) = \mu_{\underline{A}}(h) = 1$, and thus, $\forall g \in G, gT(\underline{A})g^{-1} = T(\underline{A})$. Consequently,

$$\forall (g,h) \in G^2, \quad \tau(g\underline{A} \bullet h\underline{A}) = \tau((gh)\underline{A}) \text{ (from b)}$$
$$= (gh)T(\underline{A}) = gT(\underline{A})hT(\underline{A}) = \tau(g\underline{A})\tau(h\underline{A}),$$

and τ is an isomorphism between $G/\underline{A}$ and $G/T(\underline{A})$. □

The following definition is motivated by the search for an extension of the properties of fuzzy subsets whose characteristic functions have the form: $\mu_{\underline{C}}(g) = e^{-\|g\mathbf{u}-\mathbf{v}\|/\sqrt{2}}$.

DEFINITION 5

Let $\underline{A}$ be a fuzzy subgroup of a group G and consider the fuzzy subsets $\underline{C}$ of G fulfilling the requirements

(i) $\underline{A} \supset \underline{C}^{-1} \bullet \underline{C}$,

(ii) $\underline{C} \supset \underline{C} \bullet \underline{A}$,

i.e.

$$\forall (g,h) \in G^2, \quad \mu_{\underline{C}}(g) \cdot \mu_{\underline{C}}(h) \leqslant \mu_{\underline{A}}(h^{-1}g) = \mu_{h\underline{A}}(g) \leqslant \frac{\mu_{\underline{C}}(g)}{\mu_{\underline{C}}(h)}.$$

($\underline{C}^{-1}$ is defined by: $\forall g \in G, \mu_{\underline{C}^{-1}}(g) = \mu_{\underline{C}}(g^{-1})$.)

NOTATIONS

The set of such fuzzy subsets is denoted as $Q_{\underline{A}}$: it contains at least the empty set and all the classes $g\underline{A}(Q_{\underline{A}} \supset G/\underline{A})$. The subset of $Q_{\underline{A}}$ of the fuzzy subsets containing at least one trivial element is denoted as $\Theta_{\underline{A}}$.

PROPOSITION 5

Let $\underline{A}$ be a fuzzy subgroup of a group G. Then $\Theta_{\underline{A}} = G/\underline{A}$. Therefore, when $\underline{C}$ contains a trivial element, the inclusions (i) and (ii) are equalities.

Proof

Let $\underline{C}$ belong to $\Theta_{\underline{A}}$. Let h be a trivial element of $\underline{C}$. Then

$$\forall g \in G, \quad \mu_{\underline{C}}(g) \cdot 1 \leqslant \mu_{\underline{A}}(h^{-1}g) = \mu_{h\underline{A}}(g) \leqslant \frac{\mu_{\underline{C}}(g)}{1}.$$

Thus,

$$\forall g \in G, \quad \mu_{\underline{C}}(g) = \mu_{h\underline{A}}(g).$$

On the other hand, it is easily checked that all classes modulo $\underline{A}$ belong to $\Theta_{\underline{A}}$ (h is a trivial element of $h\underline{A}$).

4. Conjugacy links

DEFINITIONS 6

Let $\underline{A}$ and $\underline{B}$ be two fuzzy subgroups of G. A fuzzy subset $\underline{C}$ of G is called a "conjugacy link between $\underline{A}$ and $\underline{B}$" if: $\underline{C} \in Q_{\underline{A}}$ and $\underline{C}^{-1} \in Q_{\underline{B}}$, i.e.

$$\text{(i)} \quad \underline{A} \supset \underline{C}^{-1} \bullet \underline{C} \quad \text{and} \quad \underline{B} \supset \underline{C} \bullet \underline{C}^{-1},$$

$$\text{(ii)} \quad \underline{C} \supset \underline{C} \bullet \underline{A} \quad \text{and} \quad \underline{C}^{-1} \supset \underline{C}^{-1} \bullet \underline{B}$$

(the empty set $\emptyset$ is always a conjugacy link).

Trivial conjugacy

DEFINITION 7

Two fuzzy subgroups $\underline{A}$ and $\underline{B}$ of a group G are said to be "trivially conjugated" if for some element g_0 of G: $g_0\underline{A} = \underline{B}g_0$.

If $\underline{A}$ and $\underline{B}$ are trivially conjugated, then their trivial parts $T(\underline{A})$ and $T(\underline{B})$ are conjugated subgroups of G.

THEOREM 2

Let $\underline{A}$ and $\underline{B}$ be two fuzzy subgroups of G. A conjugacy link with a trivial element, $\underline{C}$, exists between $\underline{A}$ and $\underline{B}$ ($\underline{C} \in \Theta_{\underline{A}}$ and $\underline{C}^{-1} \in \Theta_{\underline{B}}$) if and only if $\underline{A}$ and $\underline{B}$ are trivially conjugated.

Proof

• Suppose that $\underline{C}$ is a non-empty conjugacy link between $\underline{A}$ and $\underline{B}$ and that $\underline{C} \in \Theta_{\underline{A}}$ (or $\underline{C}^{-1} \in \Theta_{\underline{B}}$). From proposition 5, $\underline{C} \in G/\underline{A}$ and $\underline{C}^{-1} \in G/\underline{B}$. Thus, there exist two elements g_0 and h_0 of G such that

$$\forall g \in G, \quad \mu_{g_0\underline{A}}(g) = \mu_{\underline{C}}(g) = \mu_{\underline{C}^{-1}}(g^{-1}) = \mu_{h_0\underline{B}}(g^{-1}).$$

When $g = h_0^{-1}$, $\mu_{g_0\underline{A}}(h_0^{-1}) = \mu_{h_0\underline{B}}(h_0)$. Therefore, $\mu_{\underline{A}}(g_0^{-1}h_0^{-1}) = \mu_{\underline{B}}(h_0^{-1}h_0) = \mu_{\underline{B}}(e) = 1$.

Now, for any element g of G,

$$\mu_{\underline{B}g_0}(g) = \mu_{\underline{B}}(gg_0^{-1}) = \mu_{\underline{B}}(gg_0^{-1}h_0^{-1}h_0) = \mu_{\underline{B}}((gg_0^{-1}h_0^{-1}h_0)^{-1}) = \mu_{\underline{B}}(h_0^{-1}(gg_0^{-1}h_0^{-1})^{-1})$$
$$= \mu_{h_0\underline{B}}((gg_0^{-1}h_0^{-1})^{-1}) = \mu_{g_0\underline{A}}(gg_0^{-1}h_0^{-1}) = \mu_{\underline{A}}(g_0^{-1}gg_0^{-1}h_0^{-1}).$$

But since $g_0^{-1}h_0^{-1}$ is a trivial element of $\underline{A}$, proposition 2 claims that

$$\mu_{\underline{A}}(g_0^{-1}gg_0^{-1}h_0^{-1}) = \mu_{\underline{A}}(g_0^{-1}g).$$

Therefore, $\mu_{\underline{B}g_0}(g) = \mu_{g_0\underline{A}}(g)$, i.e. $\underline{A}$ and $\underline{B}$ are trivially conjugated.

• In contrast, it is easily checked that if $\underline{A}$ and $\underline{B}$ are trivially conjugated by an element g_0 of G, then the fuzzy subset $\underline{C} = g_0\underline{A} = \underline{B}g_0$ is a conjugacy link between $\underline{A}$ and $\underline{B}$ containing the trivial element g_0.

Fuzzy conjugacy

Definition 6 allows the conjugacy concept to be extended when the conjugacy link $\underline{C}$ does not contain any trivial element.

Provided that a definition of the cardinality of a fuzzy subset is given, let us define the positive real number: $X = (\#\underline{C})^2/(\#\underline{A}\#\underline{B})$.

Then, $X = 0$ only if $\underline{C} = \emptyset$. And if $\underline{C}$ contains a trivial element, i.e. if $\underline{A}$ and $\underline{B}$ are trivially conjugated, then $X = 1$. X is a measure of the extended conjugacy, but in order to be fully consistent, this measure must satisfy

(a′) $0 \leqslant X \leqslant 1$.

(b′) • $X = 0 \Leftrightarrow \underline{C} = \emptyset$.
• $X = 1 \Leftrightarrow \underline{C} \neq \emptyset$ and $\underline{A}$ and $\underline{B}$ are trivially conjugated.

The consistency of this measure depends on the definition of $\#\underline{A}$, $\#\underline{B}$, $\#\underline{C}$.

5. Connection with pairing products

DEFINITION 8

Let G be a finite or compact group, endowded with a Haar measure dg. Let $\underline{A}$ be a fuzzy subset (resp. subgroup) of G, and let p be a positive number. The "index of $\underline{A}$ in G" is defined as the positive number

$$[G: \underline{A}] = \left[\int_G e^{-p \ln^2 \mu_{\underline{A}}(g)} \, dg \right]^{-1} .$$

If G is a finite group of order $|G|$, the number of elements of $\underline{A}$ can then be defined as $\#\underline{A} = |G|/[G: \underline{A}]$.

Instead of the classical Hamming distance between fuzzy subsets of G,

$$d_H(\underline{A}, \underline{B}) = \left[\int_G |\mu_{\underline{A}}(g) - \mu_{\underline{B}}(g)|^p \, dg \right]^{1/p}, \quad 1 \leqslant p,$$

the following distance is considered:

$$d_F(\underline{A}, \underline{B}) = \left[\int_G |e^{-\ln^2 \mu_{\underline{A}}(g)} - e^{-\ln^2 \mu_{\underline{B}}(g)}|^p \, dg \right]^{1/p}$$

and the "index of $\underline{A}$ in G" is defined by $[G: \underline{A}] = [d_F(\emptyset, \underline{A})]^{-p}$.

The reason for this change has been discussed in the introduction: it is easily checked that the functions μ_{11} and μ_{22} related to the skeletal analogs $\mathbf{u}_1$ and $\mathbf{u}_2$ are membership functions of two fuzzy subgroups $\underline{A}_1$ and $\underline{A}_2$ describing the topographical symmetry of $\mathbf{u}_1$ and $\mathbf{u}_2$. On the other hand, the function μ_{12} is easily proven to be the membership function of a conjugacy link $\underline{C}$ between $\underline{A}_1$ and $\underline{A}_2$. The use of the distance d_F with $p = -a/r^q kT > 0$ allows the chemical pairing constant K to be defined as the reciprocal of the conjugacy index X:

$$X = 1/K .$$

Consequently, the requirements (a′) and (b′) for X are respectively equivalent to the requirements (a) and (b) for K.

6. Discussion

Two skeletal analogs represented by molecular vectors $\mathbf{u}_1$ and $\mathbf{u}_2$ exhibit the same symmetry if their symmetry groups are conjugated in the skeletal symmetry group G. Since $\mathbf{u}_1$ and $\mathbf{u}_2$ describe molecular topographies, informations about their respective symmetries are complemented by the consideration of the so-called symmetry subgroups $\underline{A}$ and $\underline{B}$: their abstract definition and first properties make them relevant extensions of the corresponding symmetry groups. The similarity of $\mathbf{u}_1$ and $\mathbf{u}_2$ can be revealed in some interaction between them, and the topographical symmetry of this interaction is no longer characterized by a fuzzy subgroup, but by a conjugacy link $\underline{C}$ between $\underline{A}$ and $\underline{B}$: the force of this link, i.e. the "topographical symmetry similarity", is characterized by the conjugacy index X, provided that X remains inside [0, 1] (only 0 or 1 being attained in trivial cases). When $\underline{A}$, $\underline{B}$ and $\underline{C}$ are non-trivial fuzzy subsets of G, the validity of the latter requirement depends on the distance selected for the definition of $\#\underline{A}$, $\#\underline{B}$ and $\#\underline{C}$: for the distance d_F devised above, X has a strong thermochemical meaning: G is realized as a skeletal symmetry point-group, and X varies in inverse ratio to the chemical pairing constant K, for which the consistency requirements (a′) and (b′) were proven in several cases [1,2].

Finally, X takes into account a specific interaction (of magnitude $\#\underline{C}$), and therefore characterizes the symmetry similarity more specifically than the distance $d_F(\underline{A}, \underline{B})$ does.

7. Conclusion

A particular property of a molecule (NMR spectrum, optical rotation, specific reactivity, etc.) can be described by different sets of ligand parameters which correspond to different levels of accuracy. Quite aside from a mathematical generality, the chemical relevance of the fuzzy subgroups depends on whether the $\mu(g)$ values calculated from different parameter sets vary as the "accuracy" of the descriptions produced ("p" being a freedom degree in the search for a fit). Then, "the fuzzy subgroup" of a parametrized chemical property would be defined by the parameter set giving the best fit. In contrast, starting from some parameter set (e.g. numbers), a better set (e.g. vectors) could be sought with the aid of the former approximate fuzzy subgroup. Such a putative process would be based on the assumption that the fuzzy symmetry group of a parametrized molecular property is a well-defined characteristic: it cannot be validated from physical principles, but it could be tested empirically. Nevertheless, this conceptual process will introduce a generality of the algebra of stereogenic pairing equilibria [10]. In addition, geometrical interpretations will be reported [11]: membership functions of a displacement group in E_2 or E_3 can be defined by

$$\mu(g) = \exp[-d(g\mathbf{u}, \mathbf{u})/\sqrt{2}],$$

where $\mathbf{u}$ represents a figure in E_n and d is the Hausdorff distance [12]. From this definition, the question of "continuous symmetry measures" could be addressed [13].

References and notes

[1] R. Chauvin, J. Phys. Chem. 96 (1992) 4701.
[2] R. Chauvin, J. Phys. Chem. 96 (1992) 4706.
[3] M.A. Johnson and G.M. Maggiora (eds.), *Concepts and Applications of Molecular Similarity* (Wiley, New York, 1990).
[4] R.L. Flurry, *Symmetry Groups* (Prentice-Hall, Englewood Cliffs, New Jersey, 1980).
[5] K. Mislow and J. Siegel, J. Am. Chem. Soc. 106 (1984) 3319;
S. Fujita, J. Am. Chem. Soc. 112 (1990) 3390;
S. Fujita, Tetrahedron 47 (1991) 31.
[6] L.A. Zadeh, Inf. Control 8 (1965) 338;
A. Kaufmann, *Introduction à la Théorie des Sous-ensembles Flous* (Masson & C^{ie}, Paris, 1973).
[7] J. Maruani and P. Mezey, P.C.R. Acad. Sci. Paris 305 (II) (1987) 1051; 306(II) (1988) 1141.
[8] M. Otto, T. George, C. Schierle and W. Wegscheider, Pure & Appl. Chem. 64 (1992) 497.
[9] K. Mislow and P. Bickart, Isr. J. Chem. 15 (1977) 1.
[10] R. Chauvin, Paper II of this series, J. Math. Chem. 16 (1994) 257.
[11] R. Chauvin, Entropy in dissimilarity and chirality measure, submitted for publication (1994).
[12] The Hausdorff distance has been used for measuring geometrical chirality: A. Rassat, C.R. Acad. Sci. Paris (II) 299 (1984) 53;
A.B. Buda, T. Auf der Heyde and K. Mislow, Angew. Chem. Int. Ed. Engl. 31 (1992) 989;
A.B. Buda and K. Mislow, J. Am. Chem. Soc. 114 (1992) 6006. An alternative approach based on the maximal overlap method has been proposed: G. Gilat, Chem. Phys. Lett. 121 (1985) 13.
[13] H. Zabrodsky, S. Peleg and D. Avnir, J. Am. Chem. Soc. 114 (1992) 7843.