

Unitary Symmetry of Atoms, Molecules and Codons.

Part 2. Theoretical Basis

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Abstract: In nuclear physics and elementary particle theory, an understanding of symmetry and associated concepts of the hierarchy of interactions play a fundamental role [1]. Thus the relative insignificance of electromagnetic and weak interactions as compared with the strong interaction of nucleons in the nucleus enables a model of the nucleus to be examined in the limit of precise symmetry of strong interactions. In such a model, the protons and neutrons become physically indistinguishable states of a nucleon, while the properties of the nucleus become invariant relative to isotopic transformations.

It is also possible to speak of the hierarchy of interactions participating in the formation of molecules. The energy of chemical bonds, which is 1-2 orders of magnitude greater than the energy of non-valent interactions, can be given as an example of "strong" interaction. Another example relates to the case when the energy of the valence interactions is much higher than the energy of intermolecular bonds in a condensed medium.

Weak interactions in chemistry are normally taken into account by introducing different perturbations into physical models. These perturbations are generally unmeasured parameters that are basically the adjustable magnitudes.

However, in the chosen class of molecules an attempt can be made to find the ratios of values of the examined parameter in which the contributions of "weak" interactions are compensated.

The search for such relationships and ratios is the purpose of this work.

Key words: group theory, symmetry groups, molecular symmetry group, invariants for molecules

Description of Molecular Symmetry in the Space of Their Parameters in Terms of the Group Theory

As the object of description we have chosen isostructural isovalent substituted polyatomic molecules with the general formula $Y_o A_j M_k R_l Q_p T_q$, where: Y_o - atoms of the carbon subgroup, or Y_o - other nuclear compounds (aromatic hydrocarbon, heteroarenes...), or Y_o - other nuclear compound, acting as a base, indivisible nucleus, bound by strong valence interactions compared with the weak interactions between the "isovalent ligands" - A, M, R, Q, T, (eg, solid catalyst), or - base component Y_o is absent altogether, as in the case of combinatorics of codons [2] or in the case of mixtures [3].

In the simplest case, we consider "isovalent ligands" A, M, R, Q, T, but under certain conditions, as "ligands" may be considered more complex atomic compounds.

Suppose there are n ordered elements (a, b, c, \dots) with similar physicochemical properties. Vector $|\Psi\rangle$ in Hilbert space of the states of the system is comparable to an atom of each of the elements. Let there be a simple continuous group of G_n transformations, the operators of which convert the given states into each other. If symmetry relative to this group is precise, the entire column (a, b, c, \dots) corresponds to a set of states of a certain single object.

Suppose that the similarity of (a) to (b) is greater than the similarity of (a) and (b) to (c), the similarity between (a), (b), and (c) is greater than that of (a), (b), and (c) to (d), etc. In this case the existence of $(n-1)$ quantummechanical operators D_i ($i = 1, \dots, n-1$) can be assumed, where D_1 distinguishes state (a) from (b), D_2 distinguishes state (c) from either of (a) and (b), etc. This means that the simple group G_n should have the rank $(n-1)$.

It is stressed that, by limiting ourselves to the sequences (a, b), (a, b, c), (a, b, c, d), etc, we should obtain subgroups of order 1, 2, 3, etc. ($G_n \supset G_{n-1} \supset G_{n-2} \dots G_2$). Here the structure of all the subgroups G_i is similar. There is a single simple group with such properties - $SU(n)$.

Assume that the elements (a, b, \dots) can form (in the presence of a certain fixed atom or molecule, or even by themselves) bound states (chemical compounds) of m elements. It is reasonable to assume that their physico-chemical characteristics should be similar. From the point of view of precise symmetry of G_n all these compounds are the base states of irreducible representation $D(G_n)$. The senior vector of this representation can be identified with the completely symmetrised tensor product of m states $|\Psi(\mathbf{a})\rangle$, i.e. in Dynkin numbers the sought representation is $(m, 0, 0, \dots, 0)$.

Suppose that vector S describes a certain physico-chemical property of compounds from irreducible presentation D . It should be expressed by a linear combination of base operators D_i , i.e. the operator D_i must comply with a vector in the weight space of representation D .

Knowing experimental data for the senior vector of the representation and $(n-1)$ base transitions ($a \rightarrow b$), ($a \rightarrow c$), ($a \rightarrow d$) ..., normalization of the operator S , the vector direction and the starting point can be fixed. Since only the base states of the space of the representation (chemical compounds) are realized, set of eigenvalues of any operator S is discrete and in the parameter space must exactly fit into the lattice sites of the weight diagram (see Fig.1). Consequently, the values of $\langle \Psi | S | \Psi \rangle$ for all other values can be calculated from the weight diagram, i.e. **they are predictable.**

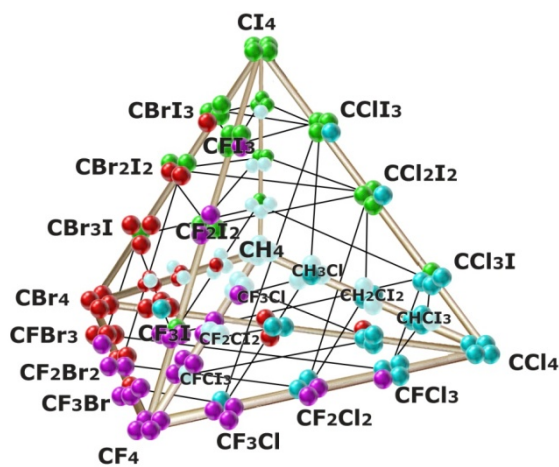


Fig. 1. The structure of the homologous series of molecules with the general formula $Y_oH_jF_kCl_mBr_nI_p$, where Y_o are the atoms of carbon subgroup or other complex atomic structure. The structure of the homologous series turned out to be the weight diagram that corresponds to the irreducible representations of the group $SU(5)$. [4]

The dimensions of weight space are fixed by the rank of the group, and for each G_n -group can be only $(n-1)$ independent physical characteristics subordinates symmetry G_n . Every other property of this kind will be expressed over $(n-1)$ "basic" properties. It is reasonable to assume that, with change to another class of molecule with the same number m , i.e. to another specimen of representation D , the nature of the dependences and direction of the "basic" vectors is retained (within the limits of precision of symmetry of G_n).

Suppose that symmetry relative to group G_n is disrupted by certain "weak" interaction. This disruption will be indicated, in particular, by the bound states (chemical compounds) having different point symmetry groups (σ). It is natural to assume that these symmetry groups reflect fairly fully the nature of disruptions.

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What is more, it can be assumed that the contributions of "weak" interaction to the matrix elements $\langle \psi_1 |S| \psi_1 \rangle$ and $\langle \psi'_1 |S| \psi'_1 \rangle$ coincide if the point symmetry groups of states $|\psi_1\rangle$ and $|\psi'_1\rangle$ coincide.

Let us examine two pairs of such states: $\psi_1 \psi'_1$ and $\psi_2 \psi'_2$ for which the differences in weight vectors are equal. Equality

$$\langle \psi_1 |S| \psi_1 \rangle - \langle \psi_2 |S| \psi_2 \rangle = \langle \psi'_1 |S| \psi'_1 \rangle - \langle \psi'_2 |S| \psi'_2 \rangle$$

will be carried out in the case of the broken symmetry, i.e., original symmetry is preserved in passing in the case of the broken symmetry, i.e., original symmetry is preserved in this type of passing $(\psi_1 \psi_2) \rightarrow (\psi'_1 \psi'_2)$.

If this assumption is valid, then the weighted space complete sets of real physical parameters will form a lattice, in which the vectors, connecting the states ψ_1 with ψ_2 and ψ'_1 with ψ'_2 are parallel and equal in absolute value.

The above views are the basis for constructing a system of linear equations, which is in violation of the selected approximation exact symmetry describes all relations on the set of the parameter in question closed class of molecules.

References

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