A SIMPLE INVERTED TREE-FLOW CHART DIAGRAM FOR POINT GROUP CLASSIFICATION

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ABSTRACT

Symmetry classification of a particular molecule into the appropriate point group plays a key role for the application of the group theory to solve chemical problems. Although there are different approaches to perform this classification, the one of an inverted tree flowchart proposed by Carter in 1968 has gone through several variations and many examples can be found in the literature. However, in some cases, simplicity has become a complex issue and the value of the original Carter's flowchart has not yet been fully acknowledged. In this paper, we introduce a new simple inverted tree flowchart and, in our approach, we state a number of questions at every point according to the presence of a particular symmetry element. Answers to five of these questions allow the student to quickly advance in the classification by reaching one out of the seven sections of the tree, which contain a great deal of information about the symmetry of the molecule under analysis.

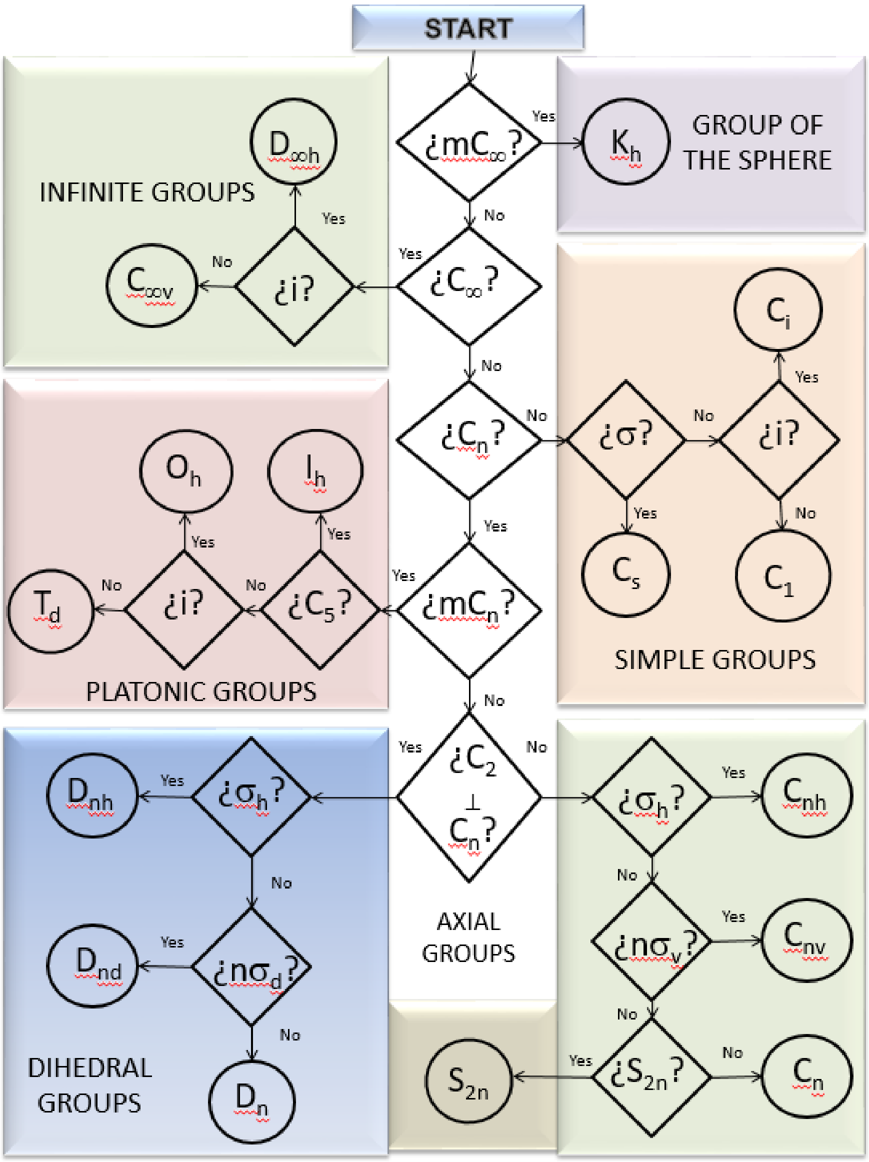
Key words: Symmetry, Point Groups, Classification Diagram, Inverted Tree

Symmetry concepts have been introduced continuously in the chemistry curriculum since the pioneering work of Cotton in 1963. These concepts were initially addressed in advanced textbooks of inorganic chemistry, especially in chapters on spectroscopy or physical methods. Currently, a description of symmetry concepts and an introduction to group theory have been included in the first chapters of most used textbooks.

To easily and quickly classify a molecular structure according to the point group which its symmetry operations belong to may represent an initial problem, but the problem is simplified if we have a guiding diagram that allows us to arrive at the correct assignments by the answers to simple questions. These questions are arranged in a logical sequence and are usually presented using a flowchart. Based on Carter's original ideas, the diagram presented here allows classifying the symmetry operations of a given molecule in the corresponding point group in a simple way. This point group consists of an inverted tree diagram presented as a flowchart, which contains five basic questions that allow access to seven sections of the tree as specified in the following table.

Section	Point Group
Group of the Sphere	K_h
Infinite Groups	$D_{\infty h}$, $C_{\infty v}$
Simple Groups	C_s, C_i, C_1
Platonic Groups	I_h, O_h, T_d
Dihedral Groups	D_{nh}, D_{nd}, D_n
Axial Groups	C_{nh}, C_{nv}, C_n
Improper Axial Group	S_{2n}

The entry to each section allows discarding a large number of specific point groups to get concentrated on simple questions that allow us to find the corresponding point group easily and quickly.



1. It starts with the question whether there are several C_∞ (mC_∞) axes. If the answer is affirmative, it will belong to the *group of the sphere* K_h.
2. If the condition above is not accomplished, one can proceed to the question whether the molecule has C_∞. If the answer is affirmative, it will belong to the *infinite groups*, and the presence of an inversion center will define whether it belongs to the point group $D_{\infty h}$ or $C_{\infty v}$.

3. If, on the contrary, the molecule does not have C_∞, the next question will be whether it has an axis of order n (C_n). If this is not the case, one will proceed to the *simple group* section, where the presence of a plane or inversion center will define whether the molecule is C_s or C_i, but if this does not occur, the molecule will belong to the point group C_1.
4. If, on the contrary, the molecule has several C_n (mC_n), it will belong to the *Platonic groups.* If it has axes of order 5, it will belong to the point group I_h, but if it does not have C_5 and has an inversion center, it will belong to the point group O_h. If this is not so, then it will belong to the point group T_d.
5. In case the molecule has an axis of a greater order C_n, the next question will be whether it has C_2 perpendicular to C_n. If this is so, the molecule will belong to the *dihedral groups*, where the presence of a horizontal or dihedral plane will define whether the molecule is D_{nh} or D_{nd}. On the other hand, if the molecule has an axis of a greater order and does not have C_2 axes perpendicular to it, the molecule will belong to the *axial groups*, and the presence of a horizontal or vertical plane will define whether the molecule belongs to the point group C_{nh} or C_{nv}. Only if the molecule has an axis of order n (C_n), then the corresponding point group will be C_n. Finally, if the molecule has an improper axis of even order (2_n), it will belong to the *improper axial point group* S_{2n}.

Thus, from five key questions, it is possible to assign one of the seven sections which the point group of a molecule can belong to and continue with simple questions to easily determine the point group that fully describes the symmetry of the molecule under analysis.

Therefore, the first step for applying group theory to understand molecular behavior is easily and quickly established through the diagram presented here. The websites suggested below allow the classification of a large number of examples.

http://symmetry.otterbein.edu/tutorial/index.html.

Last consulted on September 9, 2017.

http://www.reciprocalnet.org/edumodules/symmetry/pointgroups/examples.html

Last consulted on September 9, 2017.

http://es.webqc.org/printable-symmetrypointgroup-d2h.html

Last consulted on September 12, 2017.

http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/Molecules.html

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