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CON-COS GROUPS AND MOLECULAR SYMMETRY

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Abstract: Con-Cos groups G are defined [3] as those groups with a proper normal subgroup N for which the cosets other than N are conjugacy classes. Molecular symmetry is the important area of chemistry where group theory has been extensively used. In this paper we have examined various symmetries of molecules based on their point groups in the light of the theory of Con-Cos groups so far developed. Some generalizations have been made which show that Con-Cos groups in general represent molecules having low symmetry.

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1. Introduction

Group theory is one of the most powerful mathematical tools used in chemical bonding, quantum chemistry and spectroscopy. It provides a tool to predict, interpret, rationalize, and often simplify complex theory and data. A group [2] is a set of elements which together with a well defined operation obey certain rules. The set of operations associated with the symmetry elements of a molecule

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constitute a group. As any symmetry operation leaves a molecule physically unchanged and with the same orientation in space, its center of mass also must remain fixed in space under all symmetry operations. Thus, all the axes and planes of symmetry of a molecule must intersect at least in one common point. Such groups are called point groups. We can classify each molecule into one of the point groups.

Recently the first author has introduced and investigated [3], [4] Con-Cos groups. Con-Cos groups G are those groups with a proper normal subgroup N for which the cosets other than N are conjugacy classes. In this paper we investigate what kind of molecules are represented by Con-Cos groups.

We first give some important results on Con-Cos groups to make this paper self contained.

2. Results on Con-Cos Groups

Definition 2.1. A finite group G is called a Con-Cos group if there exists a proper normal subgroup N in G such that $xN = \mathrm{cl}\,(x)$ for all $x \in G \setminus N$.

Theorem 2.2. *If G is a Con-Cos group and N is the normal subgroup as in the above definition then $N = G'$, the derived subgroup of G.*

Theorem 2.3. *We first show that G/N is Abelian, so that $G' \subseteq N$. Let $x, y \in G$. If $x \in N$ then $xN = N$, hence yN commutes with xN. If x is not in N then $y^{-1}xy$ is not in N. In this case, we have $(y^{-1}N)(xN)(yN) = y^{-1}xyN = \mathrm{cl}\,(y^{-1}xy) = \mathrm{cl}\,(x) = xN$, so that xN and y commute with each other.*

Conversely, let $n \in N$ and $x \in G \setminus N$. Then, $xn \in \mathrm{cl}\,(x)$, so that there exists $y \in G$ such that $xn = y^{-1}xy$. Hence, $n = [x, y]$, and $n \in G'$

Theorem 2.4. *Let G be a Con-Cos group. Then $G' = \{[x, y] : y \in G\}$, for any $x \in G \setminus N$. In particular, any element of G' is a commutator.*

Theorem 2.5. *In the above proof we have shown that $G' \subseteq N$, and then that each element of N is a commutator $[x, y]$, where x is arbitrarily fixed in $G \setminus N$.*

An Abelian group is trivially a Con-Cos group with $N = \{1\}$. A general and important first result about non-Abelian Con-Cos groups is that the center is included in the derived subgroup.

Theorem 2.6. *If G is a non-Abelian Con-Cos group then $Z(G) \subseteq G'$.*

Theorem 2.7. *Let $a \in Z(G)$ and $a \neq 1$. Then* $\mathrm{cl}\,(a) = \{a\}$. *If a is not in G' then $aG' = \mathrm{cl}\,(a)$, so that $\mid G' \mid= 1$, contrary to the assumption that G is not Abelian.*

3. Examples of Non-Trivial Con-Cos Groups

Example 3.1. Consider $S_3 = \{1, a, a^2, b, ab, a^2b\}$ described via generators a, b with relations $a^3 = 1, b^2 = 1, ba = a^{-1}b$. We chose $N = \{1, a, a^2\} = \{1\} \cup \mathrm{cl}\,(a)$. Then $G/N = \{N, \{b, ab, a^2b\}\} = \{N, Nb\} = \{N, \mathrm{cl}\,(b)\}$. Thus, S_3 is a Con-Cos.

Example 3.2. Consider the dihedral group $D_4 = \{1, a, a^2, a^3, b, a^2b, ab, a^3b\}$ with relations $a^4 = 1, b^2 = 1, ba = a^{-1}b$. We choose $N = \{1\} \cup \mathrm{cl}\,(a^2) = \{1, a^2\}$. Then $D_4/N = \{N, Nb, Nab, Na\} = \{N, \mathrm{cl}\,(b), \mathrm{cl}\,(ab), \mathrm{cl}\,(a)\}$. Thus D_4 is a Con-Cos group.

Example 3.3. Consider the alternating group;

$A_4 = \{1, c, c^2, a, b, ab, ca, cb, cab, c^2a, c^2b, c^2ab\}$. We can choose $N = \{1\} \cup \mathrm{cl}\,(a) = \{1, a, b, ab\}$. Then $A_4/N = \{N, Nc, Nc^2\} = \{N, \mathrm{cl}\,(c), \mathrm{cl}\,(c^2)\}$. Hence A_4 is a Con-Cos group.

Example 3.4. Quaternion group Q is described via generators a, b with relations $a^4 = 1, b^2 = a^2, ba = a^{-1}b$ is $Q = \{1, a, a^2, a^3, b, ab, a^2b, a^3b\}$. We choose $N = \{1\} \cup \mathrm{cl}\,(a^2) = \{1, a^2\}$. Then $Q/N = \{N, Na, Nb, Nab\}\{N, \mathrm{cl}\,(a), \mathrm{cl}\,(b), \mathrm{cl}\,(ab)\}$ Thus Q is a Con-Cos group.

Example 3.5. Frobenius group of order 42 is $F_{42} = Z_7 \rtimes Z_6$ a semidirect product of Z_7 by Z_6 with Frobenius kernel $N = Z_7$. This is a Con-Cos group with $N = Z_7$.

Example 3.6. Let G be the semidirect product of Z_p and $\mathrm{Aut}\,(Z_p)$. Since Z_p is cyclic $\mathrm{Aut}\,(Z_p)$ is also cyclic. Hence each coset of Z_p in G equals to a conjugacy class in G. Thus $G = Z_p \rtimes \mathrm{Aut}\,(Z_p)$ is a Con-Cos group.

Example 3.7. Frobenius groups of order $p^\alpha(p^\alpha - 1)$ having Frobenius kernel of order p^α an elementary Abelian group are Con-Cos groups.

Remark. Note that S_3, A_4 and Examples 3.5, 3.6 and 3.7 are Frobenius groups with N as Frobenius kernel. D_4 is a semidirect product as $D_4 = Z_4 \rtimes Z_2$ and D_4 is a Con-Cos group with normal subgroup $N = \{1, a^2\}$ but the normal subgroup N is not Z_4 the kernel of the semidirect product.

Example 3.8. Dihedral group D_3 is a Con-Cos group.

Consider the dihedral group $D_3 = \{\sigma_1, \sigma_2, \sigma_3, \tau, \tau\sigma_2, \tau\sigma_3\}$, where $\sigma_1, \sigma_2, \sigma_3$ are the rotations and τ denotes the reflection. Here, $\text{cl}(\sigma_2) = \{\sigma_2, \sigma_3\}$. Now, $N = \{\sigma_1, \sigma_2, \sigma_3\} = \text{cl}(\sigma_1) \cup \text{cl}(\sigma_2)$ is the required normal subgroup.

Example 3.9. Dihedral group D_7 is a Con-Cos group.

Consider the Dihedral group $D_7 = \{e, a, ab, ab^2, ab^3, ab^4, ab^5, ab^6, b, b^2, b^3, b^4, b^5, b^6\}$. Then, $\text{cl}(b) = \{b, b^6\}$, $\text{cl}(b^2) = \{b^2, b^5\}$,$\text{cl}(b^3) = \{b^3, b^4\}$. Also, $\text{cl}(a) = \{a, ab, ab^2, ab^3, ab^4, ab^5, ab^6\}$.

Consider the set $\{b, b^2, b^3, b^4, b^5, b^6\}$. Then $N = \{e, b, b^2, b^3, b^4, b^5, b^6\} = \text{cl}(e) \cup \text{cl}(b) \cup \text{cl}(b^2) \cup \text{cl}(b^3)$ is the required normal subgroup.

Theorem 3.10. *Dihedral group D_p (p a prime) is a Con-Cos group such that N is a cyclic group of prime order.*

Proof. Consider a dihedral group D_p, where p is prime. Now D_p will have only elements of order 2 and elements of order p. Set of elements of order p with e will form the required normal subgroup. Hence D_p will be a Con-Cos group. □

Thus D_p (p a prime) are special type of Con-Cos groups in which the normal subgroup N is a cyclic group of prime order.

4. Molecular Point Groups

4.1. Molecules with Low Symmetry

These types of molecules possess either no symmetry element(except the identity elements E) or only one characteristic element: a rotation (C_n) or a reflection in a center (i) or in a mirror plane (σ). In particular:

Point Group C_1: This group has no symmetry element except the identity E. This can also be considered as a one fold proper rotation where $C_1 = E$. This type includes all the molecules possessing one asymmetric atom (C, N, P, S_i, etc.). This is clearly a Con-Cos group.

Point Groups C_n: These groups have only n fold rotation axis ($n = 1, 2, ...$) such that $C_n^n = E$. Such molecules even if symmetric possess a non-super imposable mirror image. These are also called dissymmetric molecules. Order of the group is n. All such groups will be cyclic groups and hence Con-Cos.

Point Groups C_s and C_i: These point groups have two elements each and hence they are Abelian and hence Con-Cos.

Point Groups S_n: The point groups S_n with n even has n elements in the group and possess a lower Symmetry. These point groups are in general cyclic groups and hence they are Con-Cos groups. When n is odd, no such case is known.

Point Groups D_n and C_{nv}: They are Con-Cos provided $n = 2^r, r \in N$ or $n = p, p$ a prime.

Point groups C_{nh}: They are cyclic and hence Con-Cos.

Point groups D_{nh}: They contain $4n$ number of symmetry operations. But it is not Con-Cos except when it is Abelian, i.e. for $n = 2$.

Point groups D_{nd}: They are not in general a Con-Cos group except when $n = 2$.

The molecules with higher symmetry have special point groups which are not Con-Cos.

5. Summary of the Molecular Point Groups and Con-Cos Groups

Type	Symbol	Generators	Order of G	Comments	Remarks
Low Sym.group	C_1	E	1	No Sym.	Con-Cos
	C_s	σ	2	-	Con-Cos
	C_i	i	2	$C_i = S_2$	Con-Cos
Axial	C_n	C_n	n	-	Con-Cos
	C_{nv}	C_n, σ_v	$2n$	$(C_{1v} = C_s)$	Con-Cos for $n = 2^m$
	C_{nh}	C_n,σ_n	$2n$	$(C_{1h} = C_s)$	Con-Cos
	S_{2h}	S_{2n}	$2n$	$S_1 = C_s$, $S_2 = i$	Con-Cos
Dihedral	D_n	C_n,C_2	$2n$		Con-Cos for $n = 2^r$
	D_{nh}	C_n,C_2,σ_h	$4n$		not Con-Cos except $n = 2$
	D_{nd}	C_n,C_2,σ_d	$4n$	$(D_{1d} = C_{2h})$	not Con-Cos except $n = 2$
Cubic	τ	C_3,C_2	12		not Con-Cos
Tetrahedral					
	τ_d	C_3,S_4	24		not Con-Cos
	τ_h	C_3,C_2,i	24		not Con-Cos
Octahedral	O	C_4,C_3	24		not Con-Cos
	O_h	C_4,C_3,i	48		not Con-Cos
Isohedral	I	C_5,C_3	60		not Con-Cos
	I_h	C_5, C_3, i	120		not Con-Cos

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