# Symmetry of $C_{240}$, $C_{260}$ and $C_{320}$ fullerenes

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In this paper, a method is described, by means of which it is possible to calculate the symmetry group of molecules. We apply the computer algebra system GAP to compute the symmetry group of $C_{240}$, $C_{260}$ and $C_{320}$ fullerenes.

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## 1. Introduction

A rigid molecule is defined as being such that the barriers between its versions are insuperable and there are no observable tunneling splittings. For non-rigid molecules, there are one or more contortional large amplitude vibrations such as inversion or internal rotation that give rise to tunneling splittings. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intramolecular dynamics which can be studied more easily resorting to group theory.

Following Y.G. Smeyers [1], the non-rigid molecule group (NRG) will be strictly defined as the complete set of the molecular conversion operations, which commute with a given nuclear Hamiltonian operator, limited to large amplitude motions. In addition, these molecular conversation operations will be expressed in terms of physical operations, such as rotations, internal rotations, inversions, similarly as in the Altmann's theory, rather than in terms of permutations and permutations-inversions [2,3].

The molecular symmetry group is first defined by Longuet-Higgins[4]. Although there have been earlier works that suggested the need for such a framework. Bunker and Papoušek[5] extended the definition of the molecular symmetry group to linear molecules using an extended molecular symmetry.

Graph theory is a branch of discrete mathematics concerned with relation, between objects. From the point of the graph theory, all organic molecular structures can be drawn as graphs in which atoms and bonds are represented by vertices and edges, respectively. A graph G is called a weighted graph if each edge e is assigned a non-negative number w(e), called the weight of e.

The symmetry of a graph means the automorphism group symmetry and it does not need to be isomorphic to the molecular point group symmetry. However, it does represent the maximal symmetry which the geometrical realization of a given topological structure may posses. Automorphisms have other advantages such as in generation nuclear spin species, NMR spectra, nuclear spin statistics in molecular spectroscopy, chirality and chemical isomerism [6-10].

An automorphism of a weighted graph G = (V,E) is a permutation g of V with the following properties: (i) for any u,v in V, g(u) and g(v) are adjacent if and only if u is adjacent to v. (ii) for each e in E, w(g(e)) = w(e). The set of all automorphism of a weighted graph G, with the operation of composition of permutations, is a permutation group on V(G), denoted Aut(G). A non-empty subset X of V(G) is called an orbit of G under the action of Aut(G), if there exists $x \in X$ such that $X = \{\alpha(x) \mid \alpha \in \mathrm{Aut}(G)\}$. G is called vertex transitive or simply transitive, if it has a unique orbit.

A permutation of the vertices of a graph belongs to its automorphism group if it satisfies $P^tAP = A$, where $P^t$ is the transpose of permutation matrix P and A is the adjacency matrix of the graph under consideration. There are n! possible permutation matrices for a graph with n vertices. However, all of them may not satisfy the mentioned equation.

Ashrafi and his co-workers [11-22] in a series of papers applied a computational method for computing symmetry of fullerenes. We continue the mentioned method to compute the symmetry of $C_{240}$, $C_{260}$ and $C_{320}$ fullerenes. Our calculations were done by computer algebra system GAP [23].

## 2. Results and discussion

In this section we first describe some notation which will be kept throughout. Suppose X is a set. The set of all permutations on X, denoted by $S_X$, is a group which is called the symmetric group on X. In the case that, X = {1, 2,…, n}, we denote $S_X$ by $S_n$ or Sym(n). Also, for a group G and a subset A of G, $\langle A \rangle$ is the subgroup of G generated by A.

Since 1990, two new families of carbon allotropes have become available for experimental study, both prepared by the simple method of arc discharge. Fullerenes are molecular cages with diameters of a few Å composed of tens to hundreds of carbon atoms. We now apply our computational approach to compute the symmetry group of fullerenes.

Using a GAP program we calculate a generating set for the automorphism group of fullerenes $C_n$, n = 240, 260 and 320. Suppose $\{X_n, Y_n, Z_n\}$ is a generating set for the automorphism groups of fullerenes $C_n$, n = 240, 320 and $\{X_{260}, Y_{260}\}$ is a generating set for the automorphism group of fullerene $C_{260}$. Our calculations give the following permutations as the symmetry of these fullerenes:

**$X_{240}$:=** (2,5)(3,4)(6,10)(7,9)(11,30)(12,29)(13,28)(14,27)(15,26)(16,25)(17,24)(18,23)(19,22)(20,21)
(32,35)(33,34)(36,40)(37,39)(41,60)(42,59)(43,58)(44,57)(45,56)(46,55)(47,54)(48,53)(49,52)
(50,51)(61,78)(62,77)(63,76)(64,75)(65,74)(66,73)(67,72)(68,71)(69,70)(79,90)(80,89)(81,88)
(82,87)(83,86)(84,85)(91,102)(92,101)(93,100)(94,99)(95,98)(96,97)(103,120)(104,119)
(105,118)(106,117)(107,116)(108,115)(109,114)(110,113)(111,112)(121,146)(122,145)
(123,150)(124,149)(125,148)(126,147)(127,144)(128,143)(129,142)(130,141)(131,140)
(132,139)(133,134)(135,138)(136,137)(151,176)(152,175)(153,180)(154,179)(155,178)
(156,177)(157,170)(158,169)(159,174)(160,173)(161,172)(162,171)(163,168)(164,167)
(165,166)(181,187)(182,188)(183,194)(184,193)(185,192)(186,191)(189,190)(197,200)
(198,199)(203,210)(204,209)(205,208)(206,207)(211,215)(212,216)(213,220)(214,219)
(217,218)(221,229)(222,230)(223,232)(224,231)(225,227)(226,228)(233,239)(234,240)
(235,237)(236,238),

**$Y_{240}$:=** (1,2)(3,5)(6,15)(7,14)(8,13)(9,12)(10,11)(16,30)(17,29)(18,28)(19,27)(20,26)(21,25)(22,24)
(31,35)(32,34)(36,60)(37,59)(38,58)(39,57)(40,56)(41,55)(42,54)(43,53)(44,52)(45,51)(46,50)
(47,49)(61,84)(62,83)(63,82)(64,81)(65,80)(66,79)(67,78)(68,77)(69,76)(70,75)(71,74)(72,73)
(85,90)(86,89)(87,88)(91,96)(92,95)(93,94)(97,120)(98,119)(99,118)(100,117)(101,116)
(102,115)(103,114)(104,113)(105,112)(106,111)(107,110)(108,109)(121,134)(122,133)
(123,138)(124,137)(125,136)(126,135)(127,132)(128,131)(129,130)(139,176)(140,175)
(141,180)(142,179)(143,178)(144,177)(145,170)(146,169)(147,174)(148,173)(149,172)
(150,171)(151,168)(152,167)(153,166)(154,165)(155,164)(156,163)(157,158)(159,162)
(160,161)(181,191)(182,192)(183,198)(184,197)(185,196)(186,195)(189,194)(190,193)
(199,200)(201,206)(202,205)(203,204)(207,215)(208,216)(209,220)(210,219)(213,218)
(214,217)(221,225)(222,226)(223,228)(224,227)(229,239)(230,240)(231,237)(232,238)
(233,235)(234,236),

**$Z_{240}$:=** (1,6,49,45,18)(2,7,50,41,19)(3,8,46,42,20)(4,9,47,43,16)(5,10,48,44,17)(11,12,13,14,15)
(21,30,52,35,39)(22,26,53,31,40)(23,27,54,32,36)(24,28,55,33,37)(25,29,51,34,38)
(56,60,59,58,57)(61,89,127,121,175)(62,90,128,122,176)(63,85,129,123,177)
(64,86,130,124,178)(65,87,131,125,179)(66,88,132,126,180)(67,81,133,107,173)
(68,82,134,108,174)(69,83,135,103,169)(70,84,136,104,170)(71,79,137,105,171)
(72,80,138,106,172)(73,143,113,99,165)(74,144,114,100,166)(75,139,109,101,167)
(76,140,110,102,168)(77,141,111,97,163)(78,142,112,98,164)(91,159,153,149,119)
(92,160,154,150,120)(93,161,155,145,115)(94,162,156,146,116)(95,157,151,147,117)
(96,158,152,148,118)(181,196,225,214,240)(182,195,226,213,239)(183,186,200,221,224)
(184,185,199,222,223)(187,197,218,208,238)(188,198,217,207,237)(189,192,227,211,210)
(190,191,228,212,209)(193,229,215,202,236)(194,230,216,201,235)(203,234,232,220,206)
(204,233,231,219,205)

**$X_{260}$:=** (1,9,10)(2,12,5)(3,13,4)(6,8,11)(14,146,30)(15,145,31)(16,151,32)(17,152,27)(18,144,36)
(19,149, 37)(20,150,33)(21,154,34)(22,155,28)(23,156,29)(24,147,39)(25,148,38)(26,153,35)
(40,185,107)(41,184,106)(42,190,112)(43,191,113)(44,183,105)(45,188,110)(46,189,111)
(47,193,115)(48,194,116)(49,195,117)(50,186,108)(51,187,109)(52,192,114)(53,160,66)
(54,165,67)(55,166,68)(56,157,69)(57,158,70)(58,159,71)(59,163,72)(60,164,73)(61,169,74)
(62,161,75)(63,162,76)(64,168,77)(65,167,78)(79,248,172)(80,249,171)(81,250,177)
(82,251,178)( 83,252,170)(84,253,175)(85,254,176)(86,255,180)(87,256,181)(88,257,182)
(89,258,173)(90,259,174)(91,260,179)(92,199,121)(93,204,126)(94,205,127)(95,196,118)
(96,197,119)(97,198,120)(98,202,124)(99,203,125)(100,208,130)(101,200,122)(102,201,123)
(103,207,129)(104,206,128)(131,239,212)(132,236,217)(133,235,218)(134,245,209)
(135,246,210)(136,240,211)(137,241,215)(138,237,216)(139,238,221)(140,247,213)
(141,242,214)(142,243,220)(143,244,219)(222,232,231)(223,233,230)(224,227,229)
(225,226,234),

**$Y_{260}$:=** (1,17,191,169,153)(2,22,194,168,148)(3,23,195,167,147)(4,14,185,166,156)
(5,15,184,165,155)(6,16,190,164,154)(7,20,189,163,150)(8,21,193,162,149)
(9,26,192,161,144)(10,18,183,160,152)(11,19,188,159,151)(12,25,187,158,145)

(13,24,186,157,146)(27,53,199,178,113)(28,54,204,181,116)(29,55,205,182,117)
(30,56,196,172,107)(31,57,197,171,106)(32,58,198,177,112)(33,59,202,176,111)
(34,60,203,180,115)(35,61,208,179,114)(36,62,200,170,105)(37,63,201,175,110)
(38,64,207,174,109)(39,65,206,173,108)(40,248,218,127,68)(41,249,217,126,67)
(42,250,216,125,73)(43,251,221,130,74)(44,252,212,121,66)(45,253,211,120,71)
(46,254,215,124,72)(47,255,214,123,76)(48,256,220,129,77)(49,257,219,128,78)
(50,258,209,118,69)(51,259,210,119,70)(52,260,213,122,75)(79,95,245,231,133)
(80,96,246,230,132)(81,97,240,229,138)(82,92,239,234,139)(83,101,247,225,131)
(84,102,242,224,136)(85,98,241,228,137)(86,99,237,227,141)(87,93,236,233,142)
(88,94,235,232,143)(89,104,244,222,134)(90,103,243,223,135)(91,100,238,226,140),

$\mathbf{X_{320}}$:= (2,5)(3,4)(6,14)(7,13)(8,12)(9,11)(10,15)(16,29)(17,28)(18,27)(19,26)(20,30)(21,24)(22,23)
(32,35)(33,34)(36,56)(37,60)(38,59)(39,58)(40,57)(41,51)(42,55)(43,54)(44,53)(45,52)(47,50)
(48,49)(61,66)(62,65)(63,64)(69,73)(70,72)(74,113)(75,114)(76,115)(77,116)(78,117)(79,118)
(80,119)(81,120)(82,121)(83,122)(84,123)(85,124)(86,125)(87,105)(88,104)(89,103)(90,102)
(91,101)(92,100)(93,106)(94,107)(95,112)(96,111)(97,110)(98,109)(99,108)(126,127)
(128,130)(129,131)(133,135)(134,136)(139,170)(140,169)(141,168)(142,167)(143,166)
(144,165)(145,171)(146,172)(147,177)(148,176)(149,175)(150,174)(151,173)(152,183)
(153,182)(154,181)(155,180)(156,179)(157,178)(158,184)(159,185)(160,190)(161,189)
(162,188)(163,187)(164,186)(191,218)(192,217)(193,221)(194,222)(195,219)(196,220)
(197,223)(198,226)(199,227)(200,224)(201,225)(202,228)(203,229)(204,248)(205,247)
(206,246)(207,245)(208,244)(209,243)(210,249)(211,250)(212,255)(213,254)(214,253)
(215,252)(216,251)(230,235)(231,234)(232,233)(238,242)(239,241)(256,261)(257,260)
(258,259)(264,268)(265,267)(269,313)(270,312)(271,311)(272,310)(273,309)(274,308)
(275,314)(276,315)(277,320)(278,319)(279,318)(280,317)(281,316)(282,300)(283,299)
(284,298)(285,297)(286,296)(287,295)(288,301)(289,302)(290,307)(291,306)(292,305)
(293,304)(294,303),

$\mathbf{Y_{320}}$:= (1,2)(3,5)(6,19)(7,18)(8,17)(9,16)(10,20)(11,14)(12,13)(21,29)(22,28)(23,27)(24,26)(25,30)
(31,35)(32,34)(36,51)(37,55)(38,54)(39,53)(40,52)(41,46)(42,50)(43,49)(44,48)(45,47)(57,60)
(58,59)(61,74)(62,75)(63,76)(64,77)(65,78)(66,79)(67,80)(68,81)(69,82)(70,83)(71,84)(72,85)
(73,86)(87,113)(88,114)(89,115)(90,116)(91,117)(92,118)(93,119)(94,120)(95,121)(96,122)
(97,123)(98,124)(99,125)(100,105)(101,104)(102,103)(108,112)(109,111)(126,166)(127,165)
(128,169)(129,170)(130,167)(131,168)(132,171)(133,174)(134,175)(135,172)(136,173)
(137,176)(138,177)(139,196)(140,195)(141,194)(142,193)(143,192)(144,191)(145,197)
(146,198)(147,203)(148,202)(149,201)(150,200)(151,199)(152,209)(153,208)(154,207)
(155,206)(156,205)(157,204)(158,210)(159,211)(160,216)(161,215)(162,214)(163,213)
(164,212)(178,183)(179,182)(180,181)(186,190)(187,189)(217,218)(219,221)(220,222)
(224,226)(225,227)(230,243)(231,244)(232,245)(233,246)(234,247)(235,248)(236,249)
(237,250)(238,251)(239,252)(240,253)(241,254)(242,255)(256,308)(257,309)(258,310)
(259,311)(260,312)(261,313)(262,314)(263,315)(264,316)(265,317)(266,318)(267,319)
(268,320)(269,300)(270,299)(271,298)(272,297)(273,296)(274,295)(275,301)(276,302)
(277,307)(278,306)(279,305)(280,304)(281,303)(282,287)(283,286)(284,285)(290,294)
(291,293),

$\mathbf{Z_{320}}$:= (1,6,50,41,18)(2,7,46,42,19)(3,8,47,43,20)(4,9,48,44,16)(5,10,49,45,17)(11,12,13,14,15)
(21,30,53,31,40)(22,26,54,32,36)(23,27,55,33,37)(24,28,51,34,38)(25,29,52,35,39)
(56,60,59,58,57)(61,126,182,169,76)(62,127,183,170,77)(63,128,179,166,74)
(64,129,178,165,75)(65,130,181,168,79)(66,131,180,167,78)(67,132,184,171,80)
(68,133,189,176,85)(69,134,188,175,82)(70,135,185,172,83)(71,136,190,177,86)
(72,137,187,174,81)(73,138,186,173,84)(87,114,153,285,209)(88,113,152,284,208)
(89,117,156,287,207)(90,118,157,286,206)(91,115,154,282,205)(92,116,155,283,204)
(93,119,158,288,210)(94,122,161,291,211)(95,123,162,294,216)(96,120,159,293,215)
(97,121,160,290,214)(98,124,163,289,213)(99,125,164,292,212)(100,144,298,273,196)
(101,143,297,274,195)(102,142,300,270,194)(103,141,299,269,193)(104,140,295,272,192)
(105,139,296,271,191)(106,145,301,275,197)(107,146,304,280,198)(108,151,307,279,203)
(109,150,306,276,202)(110,149,303,281,201)(111,148,302,278,200)(112,147,305,277,199)
(217,243,309,256,231)(218,244,308,257,230)(219,245,312,258,234)(220,246,313,259,235)
(221,247,310,260,232)(222,248,311,261,233)(223,249,314,262,236)(224,250,317,263,239)
(225,251,318,264,240)(226,252,315,265,237)(227,253,316,266,238)(228,254,319,267,241)
(229,255,320,268,242)

## 3. Concluding remarks

The small group library of GAP contains the structure and character table of all groups with order ≤ 2000 except from 1024, groups of order $5^5$, $7^4$ and groups of orders $p^2q$ and pqr, where p, q and r are primes. Thus GAP is very useful for research and education in chemistry.

We prove that there are several examples which show that the symmetry group of a molecule is depended critically to our accuracy in computing the Cartesian coordinates of atoms in the molecule under consideration.

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