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Group Theoretical Treatment of Substituted Saturated Fullerenes ($C_{20}H_{20-n}X_n$)

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Abstract

An Investigation of the effects of various homosubstitutions on the symmetry group of saturated fullerene ($C_{20}H_{20-n}X_n$) has been done. In substituted saturated fullerene ($C_{20}H_{20}$), tri and tetra substitutions in carbons within one hemisphere reduces the point group to Cs, whereas mono, di & penta substitutions at adjacent vertices within one hemisphere give C_{3v}, C_{2v}, and C_{5v}, respectively. It has been found that di substitution in both hemispheres give the highest degree of symmetry.

Introduction

Fullerenes are graphitic cage structures incorporating exactly twelve pentagons. The smallest possible fullerene is thus C_{20}, which consists of twelve pentagons but no hexagons. But the extreme curvature and reactivity of this structure have led to doubt about its existence and stability. Buckminster fullerene (C_{60}) having definite geometry was discovered in 1985. It has got 12 pentagonal faces and 20 hexagonal faces fused together to give a soccer-ball shape commonly called a bucky ball.[1]

Fullerene 60 has got 174 normal modes of vibration and there are 12500 resonance structures.[2] The symmetry group of C_{20} is isomorphic to the symmetry group of C_{60}. In case of substituted saturated fullerene $C_{60}H_{60-n}X_n$, the best symmetry achievable four homosubstituents is D_{2h}.[3]

Literature survey indicates that no research regarding the effect of substitution on the symmetry of saturated fullerene (C_{20}-$H_{20-n}X_n$) has been done. In this time, we are interested to study the group theoretical behavior of $C_{20}H_{20-n}X_n$ towards certain selected substitutions.

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Experimental Methods

To study the various symmetry elements present in the ($C_{20}H_{20-n}X_n$ where as n=1-5) molecules, a model was constructed. The smallest fullerene C_{20} was constructed by fusing 12 pentagons made up of hard paper. The labeling of the vertices was done following the Schlegel diagram.[4] Symmetry operations (rotation, reflection, improper reflection) were performed on the molecule $C_{20}H_{20-n}X_n$ following standard practice and it was verified whether the operations follow the rules of the group and point group standard method described elsewhere.[2]

Results and Discussion

The effect of various homosubstitutions on the symmetry group of substituted saturated fullerene ($C_{20}H_{20}$) is listed in Table 1. Mono, di and penta substitution in one hemisphere increases the symmetry elements while tri & tetra substitutions destroy the symmetry. Further di substitution in both hemisphere enhances the symmetry elements to D_{3h} whereas tetra substitution to D_{2h}. The general conclusion obtained from this study is that betterment in symmetry is achieved in the case of disubstitution in both hemisphere.

Table 1: Effects of Substitutions on the Symmetry of Saturated Fullerene ($C_{20}H_{20-n}X_n$).

	Substitution in one hemisphere					Substitution in both hemisphere		
	mono	di	tri	tetra	penta	di	tri	tetra
	1-	1,2-	1,2,3-	1,2,3,4-	1,2,3,4,5	1,18-	1,2,19-	1,2,19,20-
		2,3-	2,3,4-	2,3,4,5-		2,19-		
		3,4-	3,4,5-					
		4,5-						
Symmetry Operation	E, C_3, C_3^2,$\sigma_{v'}$, $\sigma_{v''}$,$\sigma_{v'''}$	E,C_2, $\sigma_{v'}$, $\sigma_{v''}$	E, σ	E, σ	E,C_5,C_5^4, C_5^3, C_5^2,5σ_v	E,C_3,C_3^2, $\sigma_{v'}$, $\sigma_{v''}$,$\sigma_{v'''}$,σ_h,C_2, C_2'',C_2''',$S_{3,3}^2$	E,C_2,$\sigma_{v'}$ $\sigma_{v''}$	E,$\sigma_{v'}$,$\sigma_{v''}$,σ_h, $C_2(1)$,$C_2(2)$,$C_2(3)$,i
Point Group	C_{3v}	C_{2v}	C_s	C_s	C_{5v}	D_{3h}	C_{2v}	D_{2h}

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