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Study of Structure of Buckminsterfullerene Using Nanotube Modellar Software

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Abstract**—** *Buckminsterfullerene is a type of fullerene with the formula of C60. It is an allotrope of carbon with a number of applications in fields of Drug delivery systems, Pharmaceuticals, targeted cancer therapies and hydrogen storage especially for applications in fuel cells and optical devices. In view of importance of Buckminsterfullerene its structure is studied by the use of nanotube modellar program and the structural data obtained is presented. XYZ-coordinates for Buckminsterfullerene were generated and with the help of integrated viewer of Nanotube Modeller, various geometries of Buckminsterfullerene were viewed. Some of these geometries include Ball stick model, wire frame model, Toggle bonds model, Toggle atoms model, cylinder or ball inserted, wire frame model, space filling model and Toggle fog model. Icosahedran geometry both as ball stick and wire frame model of structure of buckminsterfullerene were viewed. Also multi walled carbon nanotube (MWNT) is generated in the viewer for Buckministerfullerene.*

I. INTRODUCTION

Buckminster-fullerene, also known as a “buckyball" is a molecule composed of 60 carbon atoms and it is an allotrope of carbon other than diamond, graphene, and graphite. Its structure of a buckyball,is very much similar to the structure as a soccer ball (English football). The name ‘Buckminster fullerene' is after the name of the scientist Buckminster Fuller who first proposed it's existence. A team of scientists working on Buckminster fullerene' received a Nobel prize in Chemistry in 1984.Initially it was discovered in small proportions in soot and later it was detected spectroscopically in the vacuum of space.

The first fullerene molecule discovered is Buckminsterfullerene and is the most common form due to its occurrence naturally and it is found in soot also in small quantities. Buckminsterfullerene is a spherical fullerene molecule with 60 carbons. It was prepared intentionally in 1985 by Harold Croto, James heath, Sean O Brien, Robert Curl and Richard Smalley at Rice University. In 1996 Croto, Curl and Smalley were awarded Nobel Prize in Chemistry for their contribution in the discovery of Buckminsterfullerene and other class of fullerenes. The name Buckminsterfullerene is a homage and is in recognition of late Richard Buckminster fuller whose geodesic dome is of similar structure[1-5].

Buckminster-fullerene being a novel molecule has a number of practical uses as a very small inert spherical projectile. It shows wave-particle duality which is a quantum phenomenon, where under certain conditions bucky balls acting as massive particles behave like a wave.

This phenomenon of wave-particle duality is confirmed through the double slit experiment where Bucky balls are fired at a wall having two thin slits in it. When the molecules of bucky ball pass through the slits they hit the detector behind. An interference pattern is obtained instead of forming a linear pattern thereby indicating that the particles were mere probabilities. This gives the idea that a 60 atom molecule Buckminster-fullerene could be represented as a wave.

Structure, Properties and Applications of Buckminsterfullerene

Buckminsterfullerene is a molecule with 60 carbons that are arranged in regular pentagons and hexagons in the form of a hollow cage C_{60} structure of Buckminsterfullerene consists of 60 carbon atoms which are linked together forming cage-like structure which is hollow. Its basic structure consists of 20 hexagons and 12 pentagons with 32 faces. Among these none of the two pentagons are sharing a vertex (Figs 1&2).

Buckminsterfullerene C_{60} molecule is very stable molecule with spherical geometry, highly resistant to conditions of high temperatures and high pressures. It can react with other species at the exposed surface and at the same time the spherical geometry is also maintained. Because of its unique structure Buckminsterfullerene possess properties which are different from that of diamond and graphite. Some of its special properties are superconductivity and ability to trap other chemicals. Any element from the periodic table can be entrapped within the hollow spacious structure of Buckministerfullerene, and at the same time those elements are not reacting with the molecule.

Its conductivity can be increased by the process of doping and by doing so they can be made electrically insulating, conducting and sometimes semiconducting or even superconducting.

Potential applications of Buckminsterfullerene include Superconductors Lubricants Catalysts due to their high reactivity Drug delivery systems, pharmaceuticals and targeted cancer therapies Hydrogen storage especially for applications in fuel cells, Optical devices, Chemical sensors, Photovoltaics, Polymer electronics such as Organic Field Effect Transistors (OFETS)

Buckminsterfullerene is also useful in Antioxidants, Polymer additives, Cosmetics, where they “mopup” free radicals, Diamonds, fullerenes have been used as precursors to produce diamond films

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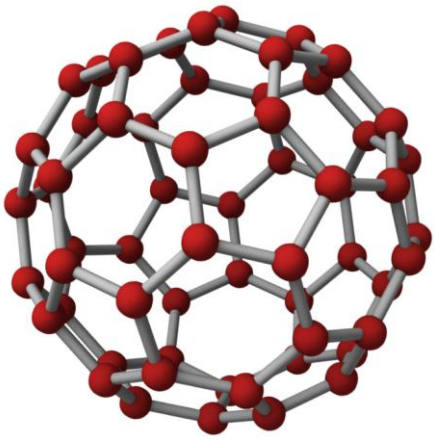


Fig. 1. 3D model image of Buckministerfullerene

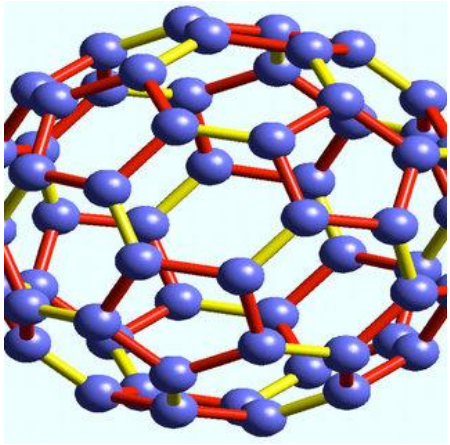


Fig. 2. Molecular structure of Buckministerfullerene

Structural data of Buckministerfullerene using chemSpider software

Molecular formula C_{60}
Average mass 720.642 Da
Monoisotopic mass 720.000000 Da
ChemSpider data 110185

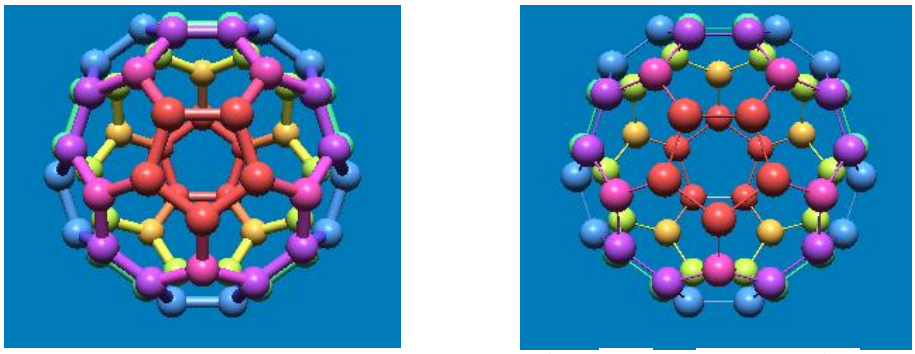
Study of Buckministerfullerene using Nanotube Modeler program

TABLE 1. XYZ-coordinates for Buckministerfullerene

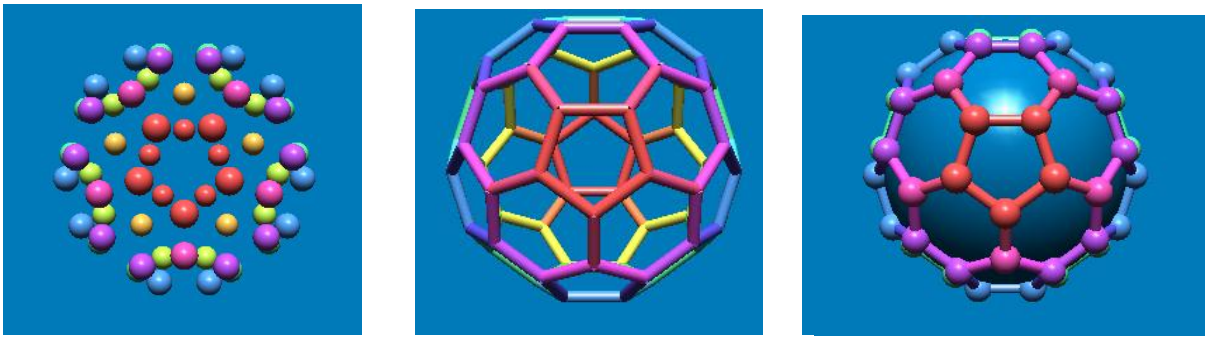
Carbon no.	Atom	X	Y	Z	Carbon no.	Atom	X	Y	Z
1	C	-0.7324	-1.0074	-3.3315	31	C	-0.7324	-3.4306	0.5885
2	C	0.7315	-1.0074	-3.3315	32	C	0.7315	-3.4306	0.5885
3	C	1.1839	0.3849	-3.3315	33	C	3.0361	-1.7562	0.5885
4	C	-0.0005	1.2453	-3.3315	34	C	3.4884	-0.3639	0.5885
5	C	-1.1844	0.3849	-3.3315	35	C	2.6081	2.3452	0.5885
6	C	-2.3044	0.7488	-2.6035	36	C	1.4238	3.2057	0.5885
7	C	-1.4244	-1.9603	-2.6035	37	C	-2.6084	2.3452	0.5885
8	C	1.4238	-1.9603	-2.6035	38	C	-1.4244	3.2057	0.5885
9	C	2.3041	0.7488	-2.6035	39	C	-3.0364	-1.7562	0.5885
10	C	-0.0005	2.4232	-2.6035	40	C	-3.4884	-0.3639	0.5885
11	C	2.6081	-1.5755	-1.8345	41	C	1.1839	-2.8079	1.8345
12	C	3.0361	-0.2586	-1.8345	42	C	2.3041	-1.994	1.8345
13	C	2.3041	1.9941	-1.8345	43	C	-2.3044	-1.994	1.8345
14	C	1.1839	2.808	-1.8345	44	C	-1.1844	-2.8079	1.8345
15	C	-1.1844	2.808	-1.8345	45	C	-3.0364	0.2587	1.8345
16	C	-2.3044	1.9941	-1.8345	46	C	-2.6084	1.5756	1.8345
17	C	-3.0364	-0.2586	-1.8345	47	C	-0.6928	2.9679	1.8345
18	C	-2.6084	-1.5755	-1.8345	48	C	0.6919	2.9679	1.8345
19	C	-0.6928	-2.9678	-1.8345	49	C	3.0361	0.2587	1.8345
20	C	0.6919	-2.9678	-1.8345	50	C	2.6081	1.5756	1.8345
21	C	-1.4244	-3.2056	-0.5895	51	C	-0.0004	-2.4231	2.6035
22	C	-2.6084	-2.3451	-0.5895	52	C	-2.3044	-0.7488	2.6035
23	C	1.4238	-3.2056	-0.5895	53	C	-1.4244	1.9604	2.6035
24	C	2.6082	-2.3451	-0.5895	54	C	1.4238	1.9604	2.6035
25	C	3.4884	0.364	-0.5895	55	C	2.3041	-0.7487	2.6035
26	C	3.0361	1.7563	-0.5895	56	C	-0.7324	1.0075	3.3315
27	C	0.7315	3.4306	-0.5895	57	C	0.7315	1.0075	3.3315
28	C	-0.7324	3.4306	-0.5895	58	C	1.1839	-0.3848	3.3315
29	C	-3.0364	1.7563	-0.5895	59	C	-0.0004	-1.2452	3.3315
30	C	-3.4884	0.364	-0.5895	60	C	-1.1844	-0.3848	3.3315

XYZ-coordinates for Buckministerfullerene were generated using the program Nanotube Modeler are given in Table 1. With the help of integrated viewer of Nanotube Modeller various geometries of Buckministerfullerene (Fig. 3) were generated and viewed[6-10]. The basis of this program is *JNanotubeApplet* by Steffen Weber[7] and further this is improved with additional features[7-10]. In this program by applying only the geometrical criteria the atomic coordinates of Buckministerfullerene were obtained and in this no energy calculations were done.

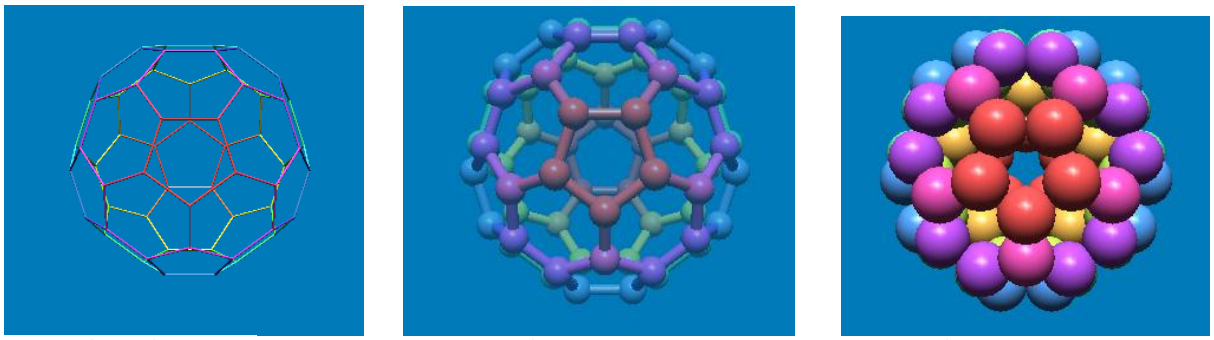
Ball stick model, wire frame model with Toggle atoms form, Toggle bonds model, Toggle atoms model, cylinder or ball inserted, wire frame model, space filling model and Toggle fog model.



(a) Ball stick model (b) wire frame model withToggle atoms form



(c) Toggle bonds model (d) Toggle atoms model (e) cylinder or ball inserted

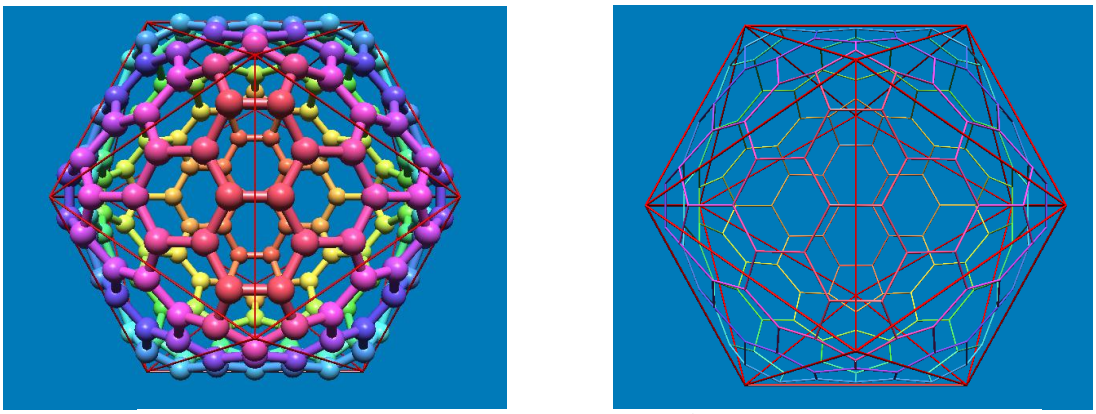


(f) wire frame model (g) space filling model (h) Toggle fog model

Fig. 3. Various models of structure of buckminsterfullerene

Icosahedran Geometry of Buckminsterfullerene

The structure of Buckminsterfullerene is a truncated icosahedron[11]. Its faces are two or more types of regular polygons. Buckminsterfullerene is made up of 20 hexagons and 12 pentagons. At the vertex of each polygon there is a carbon atom and a bond along a each polygon edge. By using the nanotube modeler the Icosahedron Geometry of Buckminsterfullerene in ball & stick and wireframe forms is obtained (Fig. 4).



ball & stick virus geometry #6 t=9 (h,k)=(3,0) wire frame virus geometry #6 t=9 (h,k)=(3,0)

Fig. 4. Icosahedran geometry of structure of buckminsterfullerene

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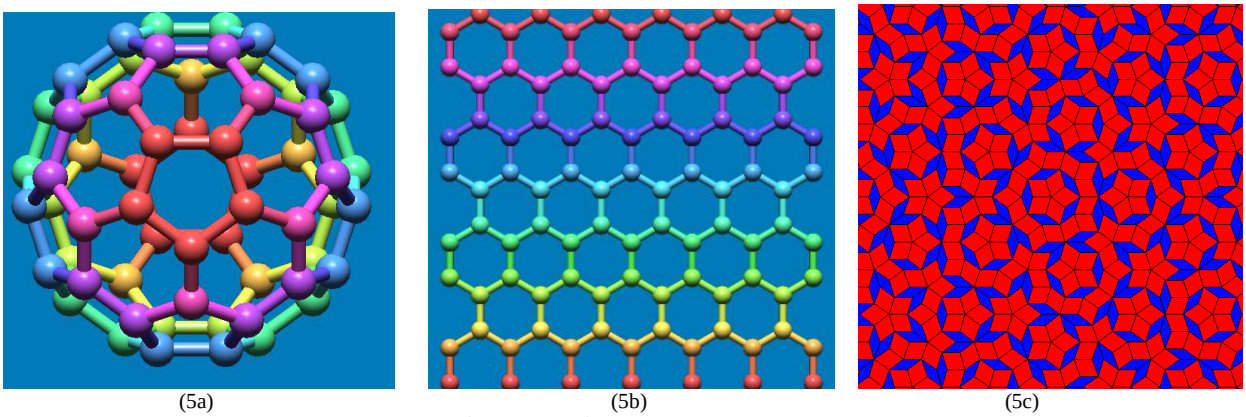
MWNT generated in the viewer for Buckministerfullerene

Bond=1.421 A From n=10 to n=70
Find MWNT sequence
Inner d=3.89 spacing=3.4 walls=5

#	(n,m)	Radius	Diameter
1	(13 , 1)	5.299	10.598
2	(20 , 4)	8.724	17.448
3	(24 , 11)	12.143	24.287
4	(33 , 11)	15.536	31.072



(5a) (5b) (5c)

Fig. 5. Structure of buckminsterfullerene obtained as multilayer graphene

Fig. 5a represents MWNT generated in the viewer for Buckministerfullerene with Atomic radius of 50% having 60 atoms and 90 bonds. Fig. 5b represents Structure of buckminsterfullerene obtained as multilayer graphene with layer width and height of 15 * 15 A band width with number of layers and distance of 2 & 3.395A respectively in the form of identical layers. Fig. 5c Structure of buckminsterfullerene obtained with nano hole array Generator (multi grid method) with tiling options of symmetry 5 , loop order 6, scale 8 and brightness 120 (with five fold symmetry 2 tile types and 705 tiles and 570 unique vertices)

II. CONCLUSION

By using the program of nanotube Modellar the structure of Buckminsterfullerene is studied and is viewed in various forms. Hence by making use of this program we can explore into structural interpretations and geometries of Buckminsterfullerene in depth.

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