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Determination of Abstract presentation of the point group of the symmetries of SF_6 molecule

¹MOLOYA BHUYAN and ²CHANDRA CHUTIA¹Department of Mathematics, Devi Charan Barua Girls' College, Jorhat-785001 (India)²Department of Mathematics, Jorhat Institute of Science & Technology, Jorhat-785010 (India)Corresponding Author E-mail: moloyabhuyan@yahoo.com, E-mail: chandra.chutia14@gmail.com<http://dx.doi.org/10.22147/jusps-B/301001>

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Abstract

The symmetry present in molecules is a fundamental concept in Chemistry. Group Theory is an extremely powerful tool which, in spite of abstractness provides the systematic treatment of symmetry of molecules that simplifies the process of obtaining a variety of information about molecules. Molecules are classified according to their symmetry properties. In this paper, analyzing all the symmetry operations as well as symmetry elements of Sulphur-hexa-fluoride (SF_6) molecule, the authors determine the point group and its abstract presentation as $\langle \alpha, \beta \mid \alpha^2 = \beta^4 = (\alpha\beta)^6 = 1 \rangle$.

Key words : molecular symmetry, octahedral geometry, symmetry elements, group presentation.
1991 Mathematics Subject Classification: 20H10, 30F10, 05C10

Introduction

Symmetry is the beauty of nature. In Greek *symmetria* means “agreement in dimension, due proportion, arrangement,” That is in as usual language it refers to a sense of harmonious and beautiful proportion and balance. In mathematics “Symmetry” has a more precise definition, that a transformation of an object is an invariant² (Artin. Pp.155-188). Molecular-symmetry, the symmetry present in molecules, is a fundamental concept in Chemistry. Group Theory is an extremely powerful tool which provides the systematic treatment of symmetry of molecules that simplifies the process of obtaining a variety of information about molecules. Molecules are classified according to their symmetry properties, *i.e.* the same set of symmetry elements grouping together⁴

(Cotton, pp.4). This classification is very important, because it allows making some general conclusions about molecular properties without any calculation. The physical properties of the molecules, such as molecular orbital, vibration modes, hybridization of atomic orbital etc. must all have the same symmetry properties as the point group to which the molecule belongs¹. The group theoretic aspects of molecular symmetry arrived in a popular form, in the middle of twentieth century. In 1929, Physicist Hans Bethe used symmetric operations as well as symmetry elements of the group of molecular symmetry in his study of Ligand field theory. From 1923-38, Hermann Weyl evolved the concept of continuous groups using matrix representations and set up the modern subject "Application of group theory to quantum mechanics". After a few years later, Hungarian chemical engineer, Eugene Wigner published his famous book, "Group theory and its application to the quantum mechanics of atomic spectra". To explain the selection rules of atomic spectroscopy, Wigner used group theory very nicely. In connection to vibrational spectra, the first character tables were compiled by Laszio Tisza in 1933. In that particular year for the first time Robert Mulliken compiled character tables in English and immediately E. Bright Wilson used them to predict the symmetry of vibrational normal modes in 1934. Rosenthal and Murphy in 1936 published the complete set of 32 crystallographic point groups¹⁰.

1. Point group of SF_6 :

Sulfur hexafluoride (SF_6) has an octahedral Geometry, consisting of six fluorine atoms attached to a central sulfur atom. Octahedral molecular geometry describes the shape of compound with six atoms or groups of atoms or ligands symmetrically arranged around a centre atom, defining the vertices of an octahedron. In geometry, an octahedron is a polyhedron with eight faces, twelve edges and six vertices. The prefix "octa" is due to the eight faces of octahedron. The term is most commonly used to refer to the regular octahedron, a platonic solid of composed of eight equilateral triangles four of which meet at each vertex⁶.

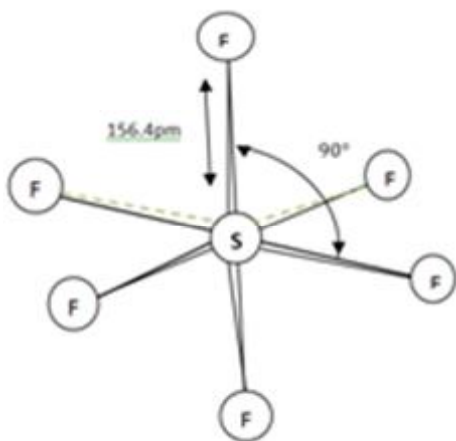


Fig. 1. Structure of SF_6 molecule

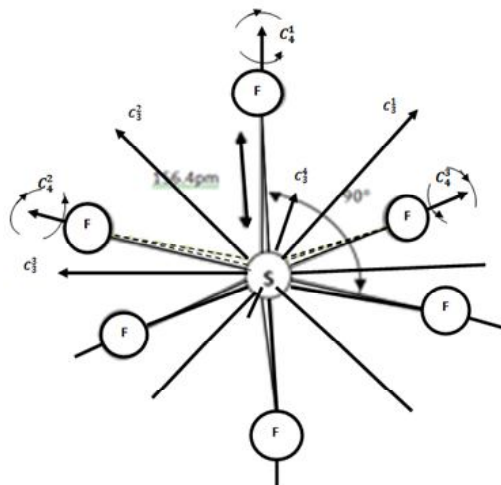


Fig. 2 : $3C_4$ Principal axes and $4C_2$ rotational axes

Sulfur hexafluoride (SF_6) possesses octahedral point group O_h (Fig. 2) of order 48 with the symmetry elements-

- 1) C_4 Principal axis with six elements $C_4^1, C_4^{-1}, C_4^2, C_4^{-2}, C_4^3, C_4^{-3}$.
- 2) One C_3 axis with eight elements $C_3^1, C_3^{-1}, C_3^2, C_3^{-2}, C_3^3, C_3^{-3}, C_3^4, C_3^{-4}$.

- 3) One C_2 axis with nine elements $C_2^1, C_2^2, C_2^3, C_2^4, C_2^5, C_2^6, C_2^7, C_2^8, C_2^9$.
- 4) Inversion center or center of symmetry i
- 5) One horizontal mirror plane with element σ_h .
- 6) Two vertical planes with elements σ_v^1 and σ_v^2 .
- 7) Six dihedral planes with elements $\sigma_d^1, \sigma_d^2, \sigma_d^3, \sigma_d^4, \sigma_d^5, \sigma_d^6$.
- 8) S_6 Improper-axis with eight elements $S_6^1, S_6^{-1}, S_6^2, S_6^{-2}, S_6^3, S_6^{-3}, S_6^4, S_6^{-4}$.
- 9) S_4 Improper axis with six elements $S_4^1, S_4^{-1}, S_4^2, S_4^{-2}, S_4^3, S_4^{-3}$.

Here the octahedral point group of sulfur Hexafluoride is defined with the notation O_h ,⁸(Somasekhara, pp.393-404) therefore

$$O_h = \{ E, 6C_4, 8C_3, 9C_2, i, \sigma_h, 2\sigma_v, 6\sigma_d, 8S_6, 6S_4 \}$$

According to the availability of the symmetry elements the molecule SF_6 possesses the point group of regular octahedron, which can be determined by the following flowchart-Fig. 3.

2. Flowchart:

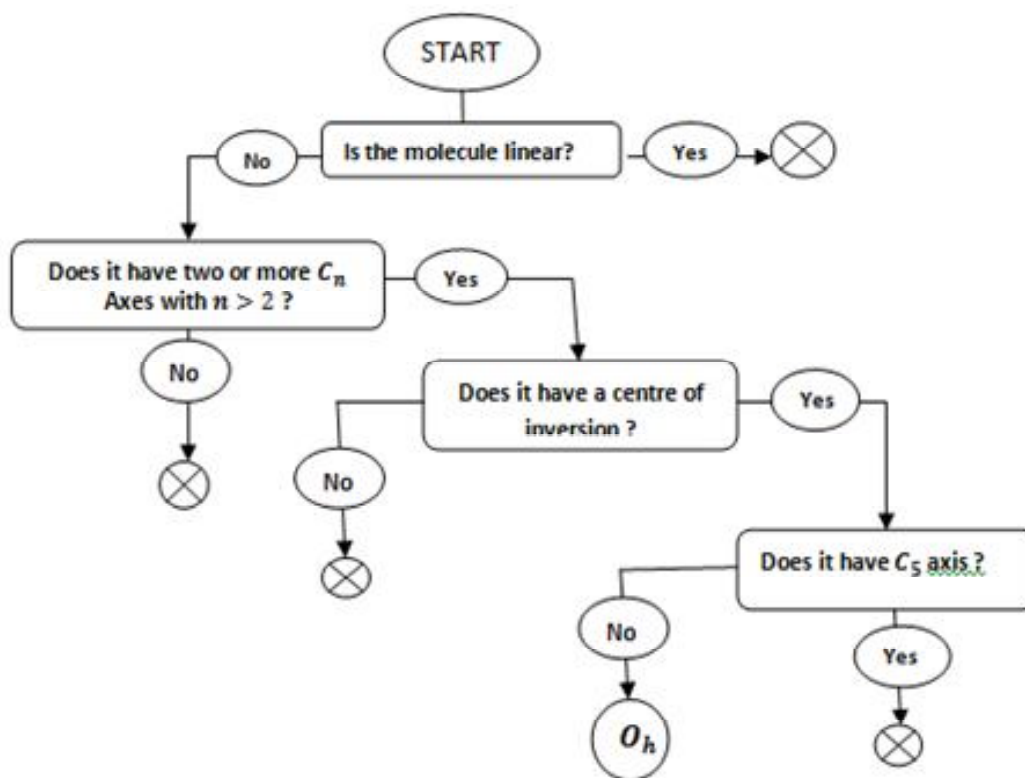


Fig. 3. Flowchart to determine point group of SF_6 molecule

3. List of symmetry elements :

Sl no	Symmetry elements	permutation	Alphabetical symbol	Sl no	Symmetry elements	permutation	Alphabetical symbol
1	E	(123456)	E	25	i	(341265)	i
2	C_4^1	(234156)	A	26	σ_h	(123465)	O
3	C_4^{-1}	(412356)	a	27	σ_v^1	(143256)	o
4	C_4^2	(625413)	B	28	σ_v^2	(321456)	P
5	C_4^{-2}	(526431)	b	29	σ_d^1	(153624)	p
6	C_4^3	(163524)	C	30	σ_d^2	(163542)	Q
7	C_4^{-3}	(153642)	c	31	σ_d^3	(432156)	q
8	C_3^1	(264531)	D	32	σ_d^4	(214356)	R
9	C_3^{-1}	(615342)	d	33	σ_d^5	(526413)	r
10	C_3^2	(536142)	F	34	σ_d^6	(625431)	S
11	C_3^{-2}	(462513)	f	35	S_6^1	(254631)	T
12	C_3^3	(254613)	G	36	S_6^{-1}	(615324)	t
13	C_3^{-3}	(516324)	g	37	S_6^2	(516342)	U
14	C_3^4	(635124)	H	38	S_6^{-2}	(264513)	u
15	C_3^{-4}	(452631)	h	39	S_6^3	(452613)	V
16	C_2^1	(341256)	J	40	S_6^{-3}	(536124)	v
17	C_2^2	(143265)	j	41	S_6^4	(635142)	W
18	C_2^3	(321465)	K	42	S_6^{-4}	(462531)	w
19	C_2^4	(361542)	k	43	S_4^1	(234165)	X
20	C_2^5	(351624)	L	44	S_4^{-1}	(412365)	x
21	C_2^6	(546213)	l	45	S_4^2	(361524)	Y
22	C_2^7	(432165)	M	46	S_4^{-2}	(351642)	y
23	C_2^8	(645231)	m	47	S_4^3	(546231)	Z
24	C_2^9	(214365)	N	48	S_4^{-3}	(645213)	z

Table 1. List of symmetry elements.

4. Group Multiplication Table:

The symmetry elements in the form of permutation, reduced to (6×6) matrix each and using matrix multiplication give the following group multiplication tables, the composition and tables are prepared and verified by using Mat lab.

Table-1

✧	<i>E</i>	<i>A</i>	<i>a</i>	<i>B</i>	<i>b</i>	<i>C</i>	<i>c</i>	<i>D</i>	<i>d</i>	<i>F</i>	<i>f</i>	<i>G</i>	<i>g</i>	<i>H</i>	<i>h</i>	<i>J</i>	<i>j</i>	<i>K</i>	<i>k</i>	<i>L</i>	<i>l</i>	<i>M</i>	<i>m</i>	<i>N</i>
<i>E</i>	<i>E</i>	<i>A</i>	<i>a</i>	<i>B</i>	<i>b</i>	<i>C</i>	<i>c</i>	<i>D</i>	<i>d</i>	<i>F</i>	<i>f</i>	<i>G</i>	<i>g</i>	<i>H</i>	<i>h</i>	<i>J</i>	<i>j</i>	<i>K</i>	<i>k</i>	<i>L</i>	<i>l</i>	<i>M</i>	<i>m</i>	<i>N</i>
<i>A</i>	<i>A</i>	<i>J</i>	<i>E</i>	<i>G</i>	<i>D</i>	<i>H</i>	<i>F</i>	<i>m</i>	<i>c</i>	<i>k</i>	<i>B</i>	<i>l</i>	<i>C</i>	<i>L</i>	<i>b</i>	<i>a</i>	<i>M</i>	<i>N</i>	<i>d</i>	<i>g</i>	<i>f</i>	<i>K</i>	<i>h</i>	<i>j</i>
<i>a</i>	<i>a</i>	<i>E</i>	<i>J</i>	<i>f</i>	<i>h</i>	<i>g</i>	<i>d</i>	<i>b</i>	<i>k</i>	<i>c</i>	<i>l</i>	<i>B</i>	<i>L</i>	<i>C</i>	<i>m</i>	<i>A</i>	<i>N</i>	<i>M</i>	<i>F</i>	<i>H</i>	<i>G</i>	<i>j</i>	<i>D</i>	<i>K</i>
<i>B</i>	<i>B</i>	<i>H</i>	<i>d</i>	<i>K</i>	<i>E</i>	<i>f</i>	<i>G</i>	<i>C</i>	<i>N</i>	<i>A</i>	<i>k</i>	<i>L</i>	<i>a</i>	<i>M</i>	<i>c</i>	<i>m</i>	<i>l</i>	<i>b</i>	<i>D</i>	<i>h</i>	<i>J</i>	<i>F</i>	<i>j</i>	<i>g</i>
<i>b</i>	<i>b</i>	<i>F</i>	<i>g</i>	<i>E</i>	<i>K</i>	<i>D</i>	<i>h</i>	<i>k</i>	<i>a</i>	<i>M</i>	<i>C</i>	<i>c</i>	<i>N</i>	<i>A</i>	<i>L</i>	<i>l</i>	<i>m</i>	<i>B</i>	<i>f</i>	<i>G</i>	<i>j</i>	<i>H</i>	<i>J</i>	<i>d</i>
<i>C</i>	<i>C</i>	<i>D</i>	<i>f</i>	<i>H</i>	<i>g</i>	<i>j</i>	<i>E</i>	<i>N</i>	<i>B</i>	<i>b</i>	<i>M</i>	<i>A</i>	<i>l</i>	<i>m</i>	<i>a</i>	<i>k</i>	<i>c</i>	<i>L</i>	<i>K</i>	<i>J</i>	<i>F</i>	<i>h</i>	<i>d</i>	<i>G</i>
<i>c</i>	<i>c</i>	<i>G</i>	<i>h</i>	<i>d</i>	<i>F</i>	<i>E</i>	<i>j</i>	<i>A</i>	<i>m</i>	<i>l</i>	<i>a</i>	<i>N</i>	<i>b</i>	<i>B</i>	<i>M</i>	<i>L</i>	<i>C</i>	<i>k</i>	<i>J</i>	<i>K</i>	<i>g</i>	<i>f</i>	<i>H</i>	<i>D</i>
<i>D</i>	<i>D</i>	<i>k</i>	<i>C</i>	<i>A</i>	<i>N</i>	<i>m</i>	<i>b</i>	<i>d</i>	<i>E</i>	<i>K</i>	<i>H</i>	<i>F</i>	<i>j</i>	<i>J</i>	<i>g</i>	<i>f</i>	<i>h</i>	<i>G</i>	<i>B</i>	<i>l</i>	<i>M</i>	<i>L</i>	<i>a</i>	<i>c</i>
<i>d</i>	<i>d</i>	<i>B</i>	<i>m</i>	<i>k</i>	<i>c</i>	<i>a</i>	<i>N</i>	<i>E</i>	<i>D</i>	<i>p</i>	<i>J</i>	<i>K</i>	<i>h</i>	<i>f</i>	<i>j</i>	<i>H</i>	<i>g</i>	<i>F</i>	<i>A</i>	<i>M</i>	<i>L</i>	<i>l</i>	<i>C</i>	<i>b</i>
<i>F</i>	<i>F</i>	<i>l</i>	<i>b</i>	<i>c</i>	<i>k</i>	<i>P</i>	<i>M</i>	<i>J</i>	<i>h</i>	<i>f</i>	<i>E</i>	<i>j</i>	<i>D</i>	<i>G</i>	<i>K</i>	<i>g</i>	<i>H</i>	<i>d</i>	<i>a</i>	<i>N</i>	<i>C</i>	<i>B</i>	<i>L</i>	<i>m</i>
<i>f</i>	<i>f</i>	<i>C</i>	<i>k</i>	<i>M</i>	<i>a</i>	<i>l</i>	<i>B</i>	<i>g</i>	<i>K</i>	<i>E</i>	<i>F</i>	<i>H</i>	<i>J</i>	<i>j</i>	<i>d</i>	<i>D</i>	<i>G</i>	<i>h</i>	<i>b</i>	<i>m</i>	<i>A</i>	<i>c</i>	<i>N</i>	<i>L</i>
<i>G</i>	<i>G</i>	<i>L</i>	<i>c</i>	<i>N</i>	<i>A</i>	<i>B</i>	<i>l</i>	<i>H</i>	<i>j</i>	<i>J</i>	<i>d</i>	<i>g</i>	<i>E</i>	<i>K</i>	<i>F</i>	<i>h</i>	<i>f</i>	<i>D</i>	<i>m</i>	<i>b</i>	<i>a</i>	<i>k</i>	<i>M</i>	<i>C</i>
<i>g</i>	<i>g</i>	<i>b</i>	<i>l</i>	<i>C</i>	<i>L</i>	<i>N</i>	<i>a</i>	<i>K</i>	<i>f</i>	<i>h</i>	<i>j</i>	<i>E</i>	<i>G</i>	<i>D</i>	<i>J</i>	<i>F</i>	<i>d</i>	<i>H</i>	<i>M</i>	<i>A</i>	<i>c</i>	<i>m</i>	<i>k</i>	<i>B</i>
<i>H</i>	<i>H</i>	<i>m</i>	<i>B</i>	<i>L</i>	<i>C</i>	<i>M</i>	<i>A</i>	<i>j</i>	<i>G</i>	<i>D</i>	<i>K</i>	<i>J</i>	<i>f</i>	<i>h</i>	<i>E</i>	<i>d</i>	<i>F</i>	<i>g</i>	<i>N</i>	<i>a</i>	<i>k</i>	<i>b</i>	<i>c</i>	<i>l</i>
<i>h</i>	<i>h</i>	<i>c</i>	<i>L</i>	<i>a</i>	<i>O</i>	<i>b</i>	<i>m</i>	<i>F</i>	<i>J</i>	<i>j</i>	<i>g</i>	<i>d</i>	<i>K</i>	<i>E</i>	<i>H</i>	<i>G</i>	<i>D</i>	<i>f</i>	<i>l</i>	<i>B</i>	<i>N</i>	<i>C</i>	<i>A</i>	<i>k</i>
<i>J</i>	<i>J</i>	<i>a</i>	<i>A</i>	<i>l</i>	<i>m</i>	<i>L</i>	<i>k</i>	<i>h</i>	<i>F</i>	<i>d</i>	<i>G</i>	<i>f</i>	<i>H</i>	<i>g</i>	<i>D</i>	<i>E</i>	<i>K</i>	<i>j</i>	<i>c</i>	<i>C</i>	<i>B</i>	<i>N</i>	<i>b</i>	<i>M</i>
<i>j</i>	<i>j</i>	<i>N</i>	<i>M</i>	<i>m</i>	<i>l</i>	<i>c</i>	<i>C</i>	<i>G</i>	<i>H</i>	<i>g</i>	<i>h</i>	<i>D</i>	<i>F</i>	<i>d</i>	<i>f</i>	<i>K</i>	<i>E</i>	<i>J</i>	<i>L</i>	<i>k</i>	<i>b</i>	<i>a</i>	<i>B</i>	<i>A</i>
<i>K</i>	<i>K</i>	<i>M</i>	<i>N</i>	<i>b</i>	<i>B</i>	<i>k</i>	<i>L</i>	<i>f</i>	<i>g</i>	<i>H</i>	<i>D</i>	<i>h</i>	<i>d</i>	<i>F</i>	<i>G</i>	<i>j</i>	<i>J</i>	<i>E</i>	<i>C</i>	<i>c</i>	<i>m</i>	<i>A</i>	<i>l</i>	<i>a</i>
<i>k</i>	<i>k</i>	<i>f</i>	<i>D</i>	<i>F</i>	<i>d</i>	<i>J</i>	<i>K</i>	<i>a</i>	<i>b</i>	<i>B</i>	<i>A</i>	<i>M</i>	<i>m</i>	<i>l</i>	<i>N</i>	<i>C</i>	<i>L</i>	<i>c</i>	<i>E</i>	<i>j</i>	<i>H</i>	<i>G</i>	<i>g</i>	<i>h</i>
<i>L</i>	<i>L</i>	<i>h</i>	<i>G</i>	<i>g</i>	<i>H</i>	<i>K</i>	<i>q</i>	<i>M</i>	<i>l</i>	<i>m</i>	<i>N</i>	<i>a</i>	<i>b</i>	<i>B</i>	<i>A</i>	<i>c</i>	<i>k</i>	<i>C</i>	<i>j</i>	<i>E</i>	<i>d</i>	<i>D</i>	<i>F</i>	<i>f</i>
<i>l</i>	<i>l</i>	<i>r</i>	<i>F</i>	<i>j</i>	<i>J</i>	<i>G</i>	<i>f</i>	<i>L</i>	<i>M</i>	<i>a</i>	<i>c</i>	<i>C</i>	<i>A</i>	<i>N</i>	<i>k</i>	<i>b</i>	<i>B</i>	<i>m</i>	<i>h</i>	<i>D</i>	<i>E</i>	<i>d</i>	<i>K</i>	<i>H</i>
<i>M</i>	<i>M</i>	<i>j</i>	<i>K</i>	<i>h</i>	<i>f</i>	<i>F</i>	<i>H</i>	<i>l</i>	<i>L</i>	<i>C</i>	<i>b</i>	<i>m</i>	<i>k</i>	<i>c</i>	<i>B</i>	<i>N</i>	<i>A</i>	<i>a</i>	<i>g</i>	<i>d</i>	<i>D</i>	<i>E</i>	<i>G</i>	<i>J</i>
<i>m</i>	<i>m</i>	<i>d</i>	<i>H</i>	<i>J</i>	<i>j</i>	<i>h</i>	<i>D</i>	<i>c</i>	<i>A</i>	<i>N</i>	<i>L</i>	<i>k</i>	<i>M</i>	<i>a</i>	<i>C</i>	<i>B</i>	<i>b</i>	<i>l</i>	<i>G</i>	<i>f</i>	<i>K</i>	<i>g</i>	<i>E</i>	<i>F</i>
<i>N</i>	<i>N</i>	<i>K</i>	<i>j</i>	<i>D</i>	<i>G</i>	<i>d</i>	<i>g</i>	<i>B</i>	<i>C</i>	<i>L</i>	<i>m</i>	<i>b</i>	<i>c</i>	<i>k</i>	<i>l</i>	<i>M</i>	<i>a</i>	<i>A</i>	<i>H</i>	<i>F</i>	<i>h</i>	<i>J</i>	<i>f</i>	<i>E</i>

Table 2: Group multiplication table-

Table -2

\star	<i>i</i>	<i>O</i>	<i>o</i>	<i>P</i>	<i>p</i>	<i>Q</i>	<i>q</i>	<i>R</i>	<i>r</i>	<i>S</i>	<i>T</i>	<i>t</i>	<i>U</i>	<i>u</i>	<i>V</i>	<i>v</i>	<i>W</i>	<i>w</i>	<i>X</i>	<i>x</i>	<i>Y</i>	<i>y</i>	<i>Z</i>	<i>z</i>
<i>E</i>	i	O	o	P	p	Q	q	R	r	S	T	t	U	u	V	v	W	w	X	x	Y	y	Z	z
<i>A</i>	x	X	q	R	v	W	P	o	u	T	Z	p	Q	z	r	Y	y	S	i	O	t	U	w	V
<i>a</i>	X	x	R	q	t	U	o	P	V	w	S	Y	y	r	z	p	Q	Z	O	i	v	W	T	u
<i>B</i>	Z	r	z	S	V	C	W	t	P	O	p	x	R	Y	y	q	X	Q	v	U	w	T	o	i
<i>b</i>	z	S	Z	r	T	w	v	U	O	P	y	V	x	Q	p	X	q	Y	W	t	u	V	i	o
<i>C</i>	y	p	Q	Y	o	O	w	u	v	t	R	z	r	X	q	Z	S	x	T	V	i	P	U	B
<i>c</i>	Y	Q	p	y	O	o	V	T	U	W	X	S	Z	R	x	r	z	q	u	w	P	i	v	t
<i>D</i>	V	T	w	u	Z	S	Y	Q	X	R	U	o	O	W	v	i	P	t	y	p	z	r	x	q
<i>d</i>	v	U	t	W	x	R	z	S	y	Q	O	w	T	P	i	V	u	o	r	Z	q	X	p	Y
<i>F</i>	t	W	v	U	X	q	r	Z	Q	y	i	T	w	o	O	u	V	P	z	S	R	x	Y	p
<i>f</i>	T	V	u	w	z	r	Q	Y	q	x	t	i	P	v	W	o	O	U	p	y	Z	S	R	X
<i>G</i>	w	u	V	T	r	z	y	p	R	X	v	O	o	t	U	P	V	W	Y	Q	S	Z	q	x
<i>g</i>	W	t	U	v	R	x	Z	r	p	Y	P	u	V	O	o	T	w	i	S	z	X	q	y	Q
<i>H</i>	U	v	W	t	q	X	S	z	Y	p	o	V	u	i	P	w	T	O	Z	r	x	R	Q	y
<i>h</i>	u	w	T	V	S	Z	p	y	x	q	W	P	i	U	t	O	o	v	Q	Y	r	z	X	R
<i>J</i>	O	i	P	o	Y	y	R	q	z	Z	w	v	W	V	u	t	U	T	x	X	p	Q	S	r
<i>j</i>	P	o	O	i	Q	p	x	X	Z	z	u	W	v	T	w	U	t	V	R	q	y	Y	r	S
<i>K</i>	o	P	i	O	y	Y	X	x	S	r	V	U	t	w	T	W	v	u	q	R	Q	p	z	Z
<i>k</i>	p	y	Y	Q	i	P	u	w	W	U	x	Z	S	q	X	z	r	R	V	T	o	O	t	v
<i>L</i>	Q	Y	y	p	P	i	T	V	t	v	q	r	z	x	R	S	Z	X	w	u	O	o	W	U
<i>l</i>	S	z	r	Z	u	V	U	v	o	i	Y	X	q	p	Q	R	x	y	t	W	T	w	P	O
<i>M</i>	R	q	X	x	W	v	O	i	w	V	z	y	Y	Z	S	Q	p	r	o	P	U	t	u	T
<i>m</i>	r	Z	S	z	w	T	t	W	i	o	O	q	X	y	Y	j	R	p	U	v	V	u	O	P
<i>N</i>	q	R	x	X	U	t	i	O	T	u	r	Q	p	S	Z	y	Y	z	P	o	W	v	V	w

Table 3: Group multiplication table-2

Table-3

✧	<i>E</i>	<i>A</i>	<i>a</i>	<i>B</i>	<i>b</i>	<i>C</i>	<i>c</i>	<i>D</i>	<i>d</i>	<i>F</i>	<i>f</i>	<i>G</i>	<i>g</i>	<i>H</i>	<i>h</i>	<i>J</i>	<i>j</i>	<i>K</i>	<i>k</i>	<i>L</i>	<i>l</i>	<i>M</i>	<i>m</i>	<i>N</i>
<i>i</i>	i	x	X	Z	z	y	Y	V	v	t	T	w	W	U	u	O	P	o	p	Q	S	R	r	q
<i>O</i>	O	X	x	S	r	Q	p	u	t	v	w	T	U	W	V	i	o	P	Y	y	Z	q	z	R
<i>o</i>	o	R	q	z	Z	p	Q	T	W	U	V	u	v	t	w	P	O	i	y	Y	r	x	S	X
<i>P</i>	P	q	R	r	S	Y	y	w	U	W	u	V	t	v	T	o	i	O	Q	p	z	X	Z	x
<i>p</i>	p	G	V	t	v	O	o	X	z	Z	x	R	r	S	q	y	Q	Y	i	P	U	w	W	u
<i>Q</i>	Q	u	w	W	U	o	O	R	S	r	q	X	Z	z	x	Y	p	y	P	i	v	V	t	T
<i>q</i>	q	o	P	V	w	v	W	Z	y	Q	r	z	Y	p	S	R	X	x	U	t	u	O	T	i
<i>R</i>	R	P	o	u	T	t	U	S	Q	y	z	r	p	Y	Z	q	x	X	W	v	V	i	w	O
<i>r</i>	r	v	U	O	P	u	V	Y	x	q	Q	c	R	X	y	Z	z	S	w	T	o	W	i	t
<i>S</i>	S	W	t	P	O	w	T	Q	R	X	Y	y	x	q	p	z	Z	r	u	V	i	v	o	U
<i>T</i>	T	y	p	R	X	S	Z	W	o	i	t	U	O	P	v	V	w	u	z	r	x	Y	q	Q
<i>t</i>	t	S	z	Y	p	x	R	O	u	T	i	P	V	w	o	W	U	v	X	q	y	Z	Q	r
<i>U</i>	U	r	Z	Q	y	R	x	P	w	V	o	O	T	u	i	v	t	W	q	X	p	z	Y	S
<i>u</i>	u	Y	Q	X	R	z	r	t	O	P	W	v	o	i	U	w	V	T	S	Z	q	y	x	p
<i>V</i>	V	p	y	x	q	r	z	v	i	o	U	t	P	O	W	T	u	w	Z	S	R	Q	X	Y
<i>v</i>	v	Z	r	p	Y	X	q	i	V	w	O	o	u	T	P	U	W	t	x	R	Q	S	y	z
<i>W</i>	W	z	S	y	Q	q	X	o	T	u	P	i	w	V	O	t	v	U	R	x	Y	r	p	Z
<i>w</i>	w	Q	Y	q	x	Z	S	U	P	O	v	W	i	o	t	u	T	V	r	z	X	p	R	y
<i>X</i>	X	i	O	T	u	W	v	z	p	Y	S	Z	Q	y	r	x	q	R	t	U	w	P	V	o
<i>x</i>	x	O	i	w	V	U	t	r	Y	p	Z	S	y	Q	z	X	R	q	v	W	T	o	u	P
<i>Y</i>	Y	w	u	v	t	i	P	x	r	S	X	q	z	Z	R	Q	y	p	O	o	W	T	U	V
<i>y</i>	y	V	T	U	W	P	i	q	Z	z	R	x	S	r	X	p	Y	Q	o	O	t	u	v	w
<i>Z</i>	Z	U	v	o	i	T	w	y	q	x	p	Q	X	R	Y	r	S	z	V	u	O	t	P	W
<i>z</i>	z	t	W	i	o	V	u	p	X	R	y	Y	q	x	Q	S	r	Z	T	w	P	U	O	v

Table 4: Group multiplication table-3

Table-4

\star	<i>i</i>	<i>O</i>	<i>o</i>	<i>P</i>	<i>p</i>	<i>Q</i>	<i>q</i>	<i>R</i>	<i>r</i>	<i>S</i>	<i>T</i>	<i>t</i>	<i>U</i>	<i>u</i>	<i>V</i>	<i>v</i>	<i>W</i>	<i>w</i>	<i>X</i>	<i>x</i>	<i>Y</i>	<i>y</i>	<i>Z</i>	<i>z</i>
<i>i</i>	<i>E</i>	J	K	j	k	L	N	M	m	l	f	F	H	h	D	d	g	G	a	A	c	C	B	b
<i>O</i>	J	<i>E</i>	j	K	c	C	M	N	b	B	G	d	g	D	h	F	H	f	A	a	k	L	l	m
<i>o</i>	K	j	<i>E</i>	J	C	c	a	A	l	m	D	H	F	G	f	g	d	h	N	M	L	k	b	B
<i>P</i>	j	K	J	<i>E</i>	L	k	A	a	B	b	h	g	d	f	G	H	F	D	M	N	C	c	m	l
<i>p</i>	k	C	c	L	<i>E</i>	j	h	G	g	H	A	B	l	N	a	b	m	M	D	f	K	J	F	d
<i>Q</i>	L	c	C	k	j	<i>E</i>	f	D	F	d	N	m	b	A	M	l	B	a	G	h	J	K	g	H
<i>q</i>	N	M	A	a	H	F	<i>E</i>	J	f	h	m	L	k	l	B	C	c	b	j	K	g	d	D	G
<i>R</i>	M	N	a	A	g	d	J	<i>E</i>	G	D	b	C	c	B	l	L	k	m	K	j	H	F	h	f
<i>r</i>	m	B	l	b	G	f	F	g	<i>E</i>	K	L	N	a	C	c	A	M	k	H	d	D	h	J	j
<i>S</i>	l	b	m	B	h	D	H	d	K	<i>E</i>	c	a	N	k	L	M	A	C	F	g	f	G	j	J
<i>T</i>	f	D	h	G	b	m	L	c	N	A	F	<i>E</i>	j	d	g	K	J	H	k	C	B	l	M	a
<i>t</i>	F	g	d	H	a	N	m	B	L	C	<i>E</i>	f	G	K	J	h	D	j	b	l	M	A	c	k
<i>U</i>	H	d	g	F	N	a	l	b	c	k	K	D	h	<i>E</i>	j	G	f	J	B	m	A	M	L	C
<i>u</i>	h	G	f	D	l	B	k	C	A	N	g	j	<i>E</i>	H	F	J	K	d	L	c	m	b	a	M
<i>V</i>	D	f	G	h	B	l	c	L	a	M	H	K	J	g	d	<i>E</i>	j	F	C	k	b	m	A	N
<i>v</i>	d	H	F	g	A	M	b	l	C	L	J	G	f	j	<i>E</i>	D	h	K	m	B	N	a	k	c
<i>W</i>	g	F	H	d	M	A	B	m	k	c	j	h	D	J	K	f	G	<i>E</i>	l	b	a	N	C	L
<i>w</i>	G	h	D	f	m	b	C	k	M	a	d	J	K	F	H	j	<i>E</i>	g	c	L	l	B	N	A
<i>X</i>	a	A	M	N	F	H	K	j	D	G	l	c	C	m	b	k	L	B	J	<i>E</i>	d	g	f	h
<i>x</i>	A	a	N	M	d	g	j	K	h	f	B	k	L	b	m	c	C	l	<i>E</i>	J	F	H	G	D
<i>Y</i>	c	L	k	C	J	K	D	f	H	g	a	l	B	M	A	m	b	N	h	G	j	<i>E</i>	d	F
<i>y</i>	C	k	L	c	K	J	G	h	d	F	M	b	m	a	N	B	l	A	f	D	<i>E</i>	j	H	g
<i>Z</i>	B	m	b	l	D	h	g	F	j	J	k	A	M	c	C	N	a	L	d	H	G	f	K	<i>E</i>
<i>z</i>	b	l	B	m	f	G	d	H	J	j	C	M	A	L	k	a	N	c	g	F	h	D	<i>E</i>	K

Table 5: Group multiplication table-4

5. Group Representation of the octahedral point group of Sulfur hexafluoride:-

(I) **Generators:** (i) $\alpha = \sigma_d^6 = S$; (ii) $\beta = C_4^3 = C$; (iii) $\alpha\beta = S_6^{-4} = W = S * C$

(II) **Presentation:-** $\alpha^2 = \beta^4 = (\alpha\beta)^6 = 1$ ⁷(Coxeter, pp.10,25)

6. List of Symmetry elements defined by the generators :

Sl no	Symmetry elements	permutation	Alphabetical symbol	Sl no	Symmetry elements	permutation	Alphabetical symbol
1	E	1	E	25	i	$(\alpha\beta)^3$	i
2	C_4^1	$\beta(\alpha\beta)^4$	A	26	σ_h	$(\alpha\beta)$	O
3	C_4^{-1}	$(\alpha\beta\alpha)$	a	27	σ_v^1	$\alpha\beta^2(\beta\alpha)^2$	o
4	C_4^2	$(\beta\alpha)^2\beta^3$	B	28	σ_v^2	$\beta^2(\alpha\beta)^3$	P
5	C_4^{-2}	$\beta^3(\alpha\beta)^2$	b	29	σ_d^1	$\alpha\beta^2(\beta\alpha)^2$	p
6	C_4^3	β	C	30	σ_d^2	$\alpha\beta^2(\alpha\beta)^2$	Q
7	C_4^{-3}	β^3	c	31	σ_d^3	$\beta^3(\alpha\beta)$	q
8	C_3^1	$\beta^2(\alpha\beta)^4$	D	32	σ_d^4	$(\beta\alpha)\beta^3$	R
9	C_3^{-1}	$(\alpha\beta\alpha)\beta^3$	d	33	σ_d^5	$\alpha\beta^2(\alpha\beta\alpha)^2$	r
10	C_3^2	$(\beta\alpha)^4$	F	34	σ_d^6	α	S
11	C_3^{-2}	$(\beta\alpha)^2$	f	35	S_6^1	$(\beta\alpha)^5$	T
12	C_3^3	$(\alpha\beta)^4$	G	36	S_6^{-1}	$\beta\alpha$	t
13	C_3^{-3}	$(\alpha\beta)^2$	g	37	S_6^2	$(\beta\alpha)\beta^2$	U
14	C_3^4	$\beta(\beta\alpha)^2\beta^3$	H	38	S_6^{-2}	$\alpha\beta(\alpha\beta\alpha)^2$	u
15	C_3^{-4}	$\beta^2(\beta\alpha)^2$	h	39	S_6^3	$\beta^2(\alpha\beta)$	V
16	C_2^1	$(\alpha\beta\alpha)^2$	J	40	S_6^{-3}	$\alpha(\beta\alpha)^4\beta^3$	v
17	C_2^2	β^2	j	41	S_6^4	$(\alpha\beta)^5$	W
18	C_2^3	$\beta^2(\alpha\beta\alpha)^2$	K	42	S_6^{-4}	$\alpha\beta$	w
19	C_2^4	$\beta(\alpha\beta\alpha)^2$	k	43	S_4^1	$\alpha(\beta\alpha)^4$	X
20	C_2^5	$\beta^3(\alpha\beta\alpha)^2$	L	44	S_4^{-1}	$(\beta\alpha)^3$	x
21	C_2^6	$\alpha(\beta\alpha)^3$	l	45	S_4^2	$\alpha(\beta\alpha)^2$	Y
22	C_2^7	$(\beta\alpha)^4\beta^3$	M	46	S_4^{-2}	$\beta(\alpha\beta)^3$	y
23	C_2^8	$\beta^2(\beta\alpha)^2\beta^3$	m	47	S_4^3	$\alpha\beta^2$	Z
24	C_2^9	$\beta^3(\alpha\beta)^4$	N	48	S_4^{-3}	$\beta^3(\alpha\beta)^5$	z

Table 6: list of symmetry elements defined by generators

7. Conclusion

Sulphur- hexa- fluoride molecule having the structure of a regular octahedron possesses the point group O_h with nine symmetry operations associated with 48 symmetry elements. So the order of the group of symmetries of Sulphur-hexa-fluoride molecule is 48 and the abstract presentation is $\langle \alpha, \beta \mid \alpha^2 = \beta^4 = (\alpha\beta)^6 = 1 \rangle$. It is observed that the point group O_h is a finite group which violets the conditions established by H.S.M.Coxeter that the “the group $(2, m, n; q)$ is finite when $\cos(2\pi/m) + \cos(2\pi/n) + \cos(\pi/q) < 1$, and m, n are either even or equal (or both); otherwise infinite”.⁵(Coxeter, pp. 74,76,93).

8. Future prospect:

The study of molecular symmetry, point group of different molecules and determination of their abstract presentation provide verification of various group theoretic aspects as well as helps to solve upper bound problem of Compact Riemann surfaces. For instance, the authors have tried to established a set of necessary and sufficient conditions for the existence of smooth epimorphism from the finite group, derived from the group of symmetries of molecule to Fuchsian group in their next paper.

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