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Computer Program for Point Group Analysis

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Symmetry and point group analysis for various molecules is one of the important parts in understanding the spectroscopic and other related properties of the substance. This is also an important portion of the curricula of the undergraduate as well as postgraduate classes. It is necessary for a student of chemistry to have a knowledge of how to locate the symmetry elements in a particular molecule and to arrive at its right point group. The present paper reports a computer program in most interactive BASIC language on Pentium IV compatible PC which can be used as teaching aid material for instructing the students.

Key Words: Computer Program, Point group.

INTRODUCTION

Symmetry properties of a molecule are more important to understand the spectroscopic and other related properties of the substance[1]. This is also an important part of the course curricula of both undergraduate and postgraduate classes. Students gets a proper grasp of various features of the analysis of point group for a molecule if they understand each and every step involving the identification of symmetry elements in the molecule.

Now-a-days, computers have a wide application in each and every field. It can be used as a tool to solve any scientific problem as well as it also helps as a teaching aid/device/machine for better interaction with students[2].

The present communication reports the program for analysis of a molecule for its correct point group in most interactive BASIC language with easy commands[3]. This can be used as an aid for instructing the students and to give a first hand knowledge. Flow chart for the program is also given in Fig. 1.

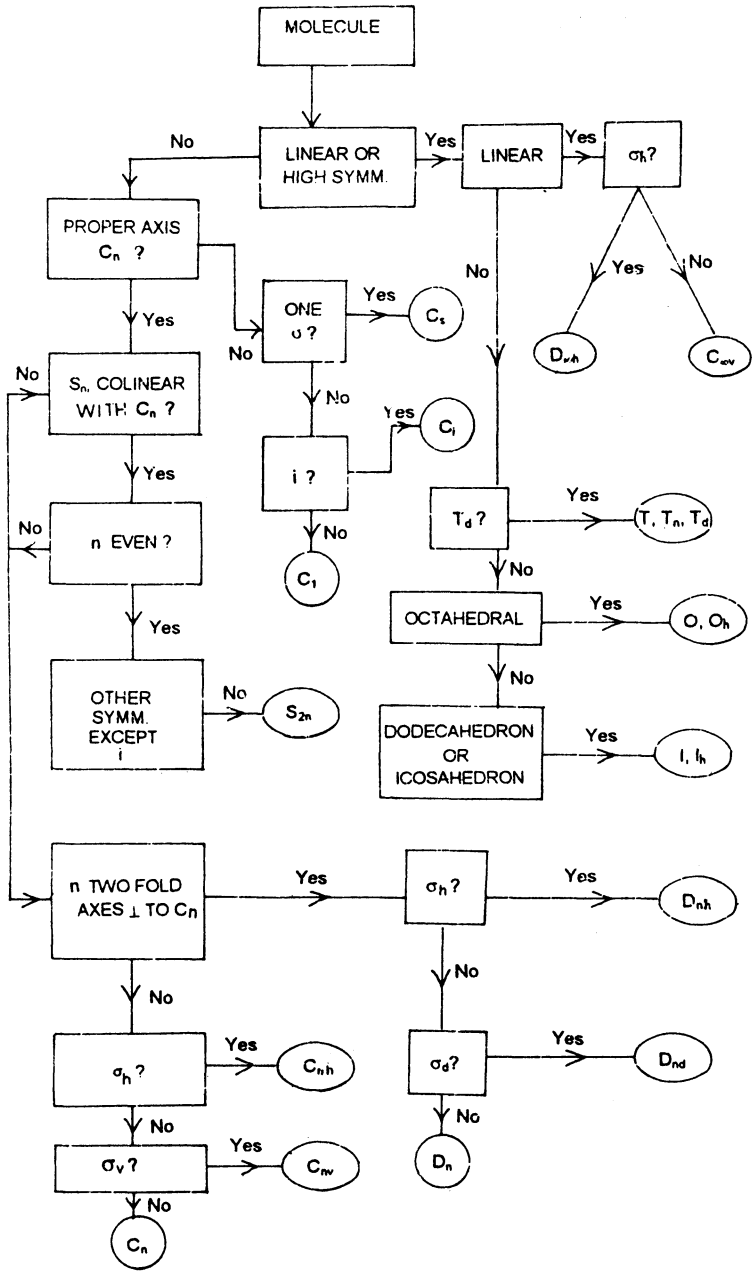

Fig. 1. Groups and Point Groups

The program is as listed below along with some outputs to rationalize it.

```
10 REM PROGRAM FOR POINT GROUP ANALYSIS OF A MOLECULE
12 PRINT "PROGRAM FOR POINT GROUP ANALYSIS"
14 PRINT "ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM"
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```
 20 PRINT "WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH
    SYMM?"
 30 INPUT A$
 40 IF A$ = "Y" THEN 45 ELSE 200
 45 PRINT "YOUR MOLECULE IS LINEAR?"
 47 INPUT C$
 48 IF C$ = "Y" THEN 50 ELSE 100
 50 PRINT "YOUR MOLECULE CONTAINS HORIZONTAL PLANE?"
 60 INPUT B$
 70 IF B$ = "Y" THEN 80 ELSE 90
 80 PRINT "POINT GROUP OF YOUR MOLECULE IS DINH"
 85 GOTO 760
 90 PRINT "POINT GROUP OF YOUR MOLECULE IS CINV"
 95 GOTO 760
100 PRINT "YOUR MOLECULE IS OF HIGH SYMMETRY TETRAHED OR
    OCTAHED OR ICOSAHED?"
110 PRINT "ENTER T FOR TERAHED O FOR OCTAHED AND I FOR
    ICOSAHED"
120 INPUT D$
130 IF D$ = "T" THEN 140 ELSE 150
140 PRINT "POINT GROUP FOR YOUR MOLECULE IS TD"
145 GOTO 760
150 IF D$ = "O" THEN 160 ELSE 170
160 print "POINT GROUP FOR YOUR MOLECULE IS OH"
165 GOTO 760
170 IF D$ = "I" THEN 180 ELSE 190
180 PRINT "POINT GROUP FOR YOUR MOLECULE IS IH"
185 GOTO 760
190 PRINT "YOU ARE JOKING"
195 GOTO 760
200 PRINT "YOUR MOLECULE CONTAINS PROPER AXIS CN?"
210 INPUT E$
220 IF E$ = "Y" THEN 230 ELSE 630
230 PRINT "YOUR MOLECULE CONTAINS SN COLINEAR WITH CN?"
240 INPUT F$
250 IF F$ = "Y" THEN 260 ELSE 300
260 PRINT "IS N EVEN?"
270 INPUT G$
280 IF G$ = "Y" THEN 290 ELSE 300
290 PRINT "POINT GROUP OF YOUR MOLECULE IS S2N"
295 GOTO 760
300 PRINT "YOUR MOLECULE CONTAINS N TWO FOLD AXES PERPEN-
    DICULAR TO CN AXIS?"
310 INPUT H$
320 IF H$ = "Y" THEN 330 ELSE 480
330 PRINT "YOUR MOLECULE CONTAINS HORIZONTAL PLANE?"
```

```
340 INPUT I$
350 IF I$ = "Y" THEN 360 ELSE 390
360 PRINT "GIVE VALUE FOR N"
370 INPUT N
380 PRINT "POINT GROUP FOR YOUR MOLECULE IS D";N;"H"
385 GOTO 760
390 PRINT "YOUR MOLECULE CONTAINS DIAGONAL PLANE?"
400 INPUT J$
410 IF J$ = "Y" THEN 420 ELSE 450
420 PRINT "GIVE VALUE FOR N"
430 INPUT N1
440 PRINT "POINT GROUP FOR YOUR MOLECULE IS D"; N1; "D"
445 GOTO 760
450 PRINT "GIVE THE VALUE FOR N"
460 INPUT N2
470 PRINT "POINT GROUP FOR YOUR MOLECULE IS D";N2
475 GOTO 760
480 PRINT "YOUR MOLECULE CONTAINS HORIZONTAL PLANE"
490 INPUT K$
500 IF K$ = "Y" THEN 510 ELSE 540
510 PRINT "ENTER THE VALUE FOR N"
520 INPUT N3
530 PRINT "POINT GROUP FOR YOUR MOLECULE IS C"; N3 : "H"
535 GOTO 760
540 PRINT "YOUR MOLECULE CONTAINS VERTICAL PLANE?"
550 INPUT L$
560 IF L$ = "Y" THEN 570 ELSE 600
570 PRINT "ENTER THE VALUE FOR N"
580 INPUT N4
590 PRINT "THE POINT GROUP FOR YOUR MOLECULE IS C";N4; "V"
595 GOTO 760
600 PRINT "ENTER THE VALUE FOR N"
610 INPUT N5
620 PRINT "POINT GROUP FOR YOUR MOLECULE IS C"; N5
625 GOTO 760
630 PRINT "YOUR MOLECULE CONTAINS ONLY ONE PLANE?"
640 INPUT M$
650. IF M$ = "Y" THEN 660 ELSE 680
660 PRINT "YOUR MOLECULE CONTAINS ONLY ONE PLANE?"
640 INPUT M$
650 IF M$ = "Y" THEN 660 ELSE 680
660 PRINT "POINT GROUP FOR YOUR MOLECULE IS CS"
670 GOTO 760
680 PRINT "YOUR MOLECULE CONTAINS INVERSION CENTRE ONLY?"
690 INPUT N$
700 IF N$ = "Y" THEN 710 ELSE 730
```

```
710 PRINT "POINT GROUP FOR YOUR MOLECULE IS CI"
720 GOTO 760
730 PRINT "YOUR MOLECULE CONTAINS NO SYMMETRY ELEMENT"
735 INPUT P$
737 IF P$ = "Y" THEN 740 ELSE 760
740 PRINT "POINT GROUP OF YOUR MOLECULE IS C1"
750 GOTO 760
760 PRINT "IS IT NOT INTERESTING TO INTERACT IN THIS WAY?"
770 PRINT "DO YOU WANT TO RUN IT AGAIN Y/N?"
780 INPUT O$
790 IF O$ = "Y" THEN 10 ELSE 800
800 END
Ok_
```

{Various symbols used in the program are: DINH = $D_{\infty h}$; CINV = $C_{\infty h}$; TETRAHED = tetrahedron; OCTAHED = octahedron; ICOSAHED = icosahedron; TD = T_d; OH = O_h; IH = I_h; CN = C_n; S2N = S_{2n}; DNH = D_{nh}; DND = D_{nd}; DN = D_n; CNH = C_{nh}; CNV = C_{nv}; CN = C_n; CS = C_s; CI = C_i; and C1 = C_1}

Output for this program is as given below:

```
RUN
PROGRAM FOR POINT GROUP ANALYSIS
ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM
WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH SYMM?
? Y
YOUR MOLECULE IS LINEAR?
? Y
YOUR MOLECULE CONTAINS HORIZONTAL PLANE?
? Y
POINT GROUP OF YOUR MOLECULES IS DINH
IS IT NOT INTERESTING TO INTERACT IN THIS WAY?
DO YOU WANT TO RUN IT AGAIN Y/N?
? Y
PROGRAM FOR POINT GROUP ANALYSIS
ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM
WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH SYMM?
? Y
YOUR MOLECULE IS LINEAR?
? N
YOUR MOLECULE IS OF HIGH SYMMETRY TETRAHED OR OCTAHED
OR ICOSAHED?
ENTER T FOR TERAHED O FOR OCTAHED AND I FOR ICOSAHED
? T
POINT GROUP FOR YOUR MOLECULE IS TD
IS IT NOT INTERESTING TO INTERACT IN THIS WAY?
DO YOU WANT TO RUN IT AGAIN Y/N?
```

```
? Y
PROGRAM FOR POINT GROUP ANALYSIS
ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM
WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH SYMM?
? Y
YOUR MOLECULE IS LINEAR?
? N
YOUR MOLECULE IS OF HIGH SYMMETRY TETRAHED OR OCTAHED
OR ICOSAHED?
ENTER T FOR TERAHED O FOR OCTAHED AND I FOR ICOSAHED
? I
POINT GROUP FOR YOUR MOLECULE IS IH
IS IT NOT INTERESTING TO INTERACT IN THIS WAY?
DO YOU WANT TO RUN IT AGAIN Y/N?
? N
OK

RUN
PROGRAM FOR POINT GROUP ANALYSIS
ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM
WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH SYMM?
? N
YOUR MOLECULE CONTAINS PROPER AXIS CN?
? Y
YOUR MOLECULE CONTAINS SN COLINEAR WITH CN?
? N
IS N EVEN
? Y
POINT GROUP OF YOUR MOLECULE IS S2N
IS IT NOT INTERESTING TO INTERACT IN THIS WAY?
DO YOU WANT TO RUN IT AGAIN Y/N?
? N
Ok_

RUN
PROGRAM FOR POINT GROUP ANALYSIS
ENTER THE ANSWERS TO THE QUESTIONS IN Y/N FORM
WHETHER YOUR MOLECULE IS LINEAR OR OF HIGH SYMM?
? N
YOUR MOLECULE CONTAINS PROPER AXIS CN?
? Y
YOUR MOLECULE CONTAINS SN COLINEAR WITH CN?
? N
YOUR MOLECULE CONTAINS N TWO FOLD AXES PERPENDICULAR TO
CN AXIS?
? Y
```

YOUR MOLECULE CONTAINS HORIZONTAL PLANE?
? Y
GIVE VALUE FOR N
? 4
POINT GROUP FOR YOUR MOLECULE IS D 4 H
IS IT NOT INTERESTING TO INTERACT IN THIS WAY?
DO YOU WANT TO RUN IT AGAIN Y/N?
? N
Ok_

Conclusion

This single and small program can be used as teaching aid material as this program works for point group analysis of a molecule and helps in better understanding of the concept to the UG or PG students.

REFERENCES

1. F.A. Cotton, Chemical Application of Group Theory, 2nd Edn., Wiley Eastern Limited (1989).
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