# 2. PROGRAMMING ORTEP

## 2.1 GENERAL PRINCIPLES

Originally, the input to ORTEP was a set of punched cards. Now, the ORTEP input is a computer text file containing lines of information corresponding to the cards. However, since the input must generally be very precisely formatted as required by the FORTRAN code, it is still convenient to refer to the individual lines of input as "cards," and that practice is maintained in this report.

For those who may be unfamiliar with FORTRAN input, two points are in order. First, when a card field is specified to contain a particular numeric input item, the value should be entered in the rightmost positions of the field. Secondly, the value of "0" is assigned to a numeric input item whose card field is left blank.

ORTEP input consists of five types of information.

- Title card (see 3.2.1)
- Cell parameter card (see 3.2.2)
- Symmetry cards (see 3.2.3)
- Atomic parameter cards (see 3.2.4)
- Instruction cards (see Table 2.1 and 3.3)

ORTEP applies the concept of programming to the task of drawing illustrations. Using this approach, a set of basic building block operations have been developed that are put together by the user to "program" an illustration. These operations, which are termed instructions, control six types of activities.

- setting up the graphics
- composing an illustration
- drawing the illustration
- repeating a sequence of other instructions
- calculating and printing tables of ancillary information
- terminating the process

Table 2.1 is a summary of the ORTEP instructions. Each instruction starts on a separate card and consists of an identifying number and the parameters needed for the particular instruction. The general role of these instructions is explained in the remaining parts of this section, and the individual instructions are described in detail in Section 3.3. The simplest way to construct the program is, first, to select a "template" instruction set used for some previous related ORTEP drawing and then to scan through the list of instructions in Table 2.1 and pick out the relevant parameters and new instructions to modify the template.

In order to produce high quality illustrations with ORTEP, an iterative approach is generally required; that is, the illustration must usually be computed and plotted several times before an optimal figure is produced. With each trial, as many factors as possible are optimized to give a more informative and more aesthetically pleasing result.

## 2.2 PROGRAMMING A NONSTEREOSCOPIC ILLUSTRATION FOR ORTEP

This section describes the general stepwise procedure to follow when writing an ORTEP program to draw a single nonstereographic illustration of the contents of one unit cell. The instruction numbers used are examples only, and often other instructions may be used instead.

### 2.2.1 Graphics Setup

The first instruction card is instruction 201 (see 3.3.3), which initializes plotting.

Next, instruction 301 (see 3.3.4.1) is needed to set the following drawing parameters: *x* dimension for the plot boundary, *y* dimension for the plot boundary, viewing distance for perspective projection (or "0" as a signal for parallel projection), and border (or margin) dimension inside the boundary. All values are supplied in inches.

### 2.2.2 Composing the Illustration

This step involves specifying which atoms are to be used as the figure subject, the rotational orientation of the figure, and the scaling and positioning of the figure relative to the drawing area. These three components of composition are implemented by the 400, 500, and 600 series instructions, respectively.

Atoms can be explicitly added to the figure with a 401 instruction (see 3.3.5.1). For unit cell content drawings, the 404 instruction (see 3.3.5.3) is useful. It defines a triclinic box of enclosure, and ORTEP determines which atoms appear in the figure.

A 501 instruction (see 3.3.6.1) can be used to orient the crystal axes relative to the *x* and *y* axes of the plot. If additional adjustment of the figure orientation is necessary, a 502 instruction (see 3.3.6.2) can be used after the 501.

Scaling and positioning of the figure to fill the drawing area can be accomplished automatically with a 604 instruction (see 3.3.7.1).

### 2.2.3 Drawing the Illustration

Crystal structure illustrations of the ball-and-stick type are made up of three components: balls (atoms), sticks (bonds), and labels. The three components are drawn with the 700, 800, and 900 instruction series, respectively; the first two instruction series can also perform certain types of labeling. Before drawing any atoms or bonds, instruction 1001 (or 511) (see 3.3.12) should be used to calculate and store the information needed for the overlap correction.

The atom representation can be either a general ellipsoid or a boundary ellipse. In some cases, these become a sphere and a circle. Chemical symbols may be plotted simultaneously with the atoms. A 704 instruction (see 3.3.8) will draw circles for all the atoms of the subject and put the chemical symbols within the circles.

Bonds are not always necessary in a drawing; but for structures with molecules or with distinctive groupings, they are usually quite helpful. The most convenient method for describing and drawing bonds is instruction 812 (see 3.3.9.2). This instruction uses vector search codes (see 3.1.5) that reflect the user's knowledge of the structural chemistry and the interatomic distance ranges for the compound being drawn. Covalent bonds or any other desired type are found and drawn automatically from the list of atoms that make up the subject. If desired, the interatomic distance label can also be drawn with the bond.

Various types of labeling can be done with the 900 series instruction. The one that will most often be included is a caption for the figure, provided by the 902 instruction (see 3.3.10).

### 2.2.4 Terminating the Drawing of the Illustration

Instruction 202 with no parameters (see 3.3.3) terminates the plotting.

To terminate ORTEP, a -1 instruction (see 3.3.13) is used as the last instruction of the input.

## 2.3 PROGRAMMING A STEREOSCOPIC ILLUSTRATION FOR ORTEP

A stereoscopic pair of figures is simply two perspective views of the subject as seen from two different viewpoints (which are usually 5°–6° apart). This pair is produced with ORTEP by programming for two drawings. A few instructions in addition to those outlined in Section 2.2 are needed for producing stereo figures. These are the stereoscopic rotation instruction 503 and the 1100 series of instructions that are used to repeat a series of instructions. A program to draw a stereo pair would involve the following steps.

1. set up the graphics
2. compose the subject
3. stereo rotate subject for left-eye view
4. store overlap information
5. draw the subject
6. shift plot origin for second view
7. stereo rotate subject for right-eye stereo view
8. store overlap information
9. draw the subject
10. terminate plotting
11. terminate ORTEP

### 2.3.1 Stereoscopic Rotations

In general, one member of a detailed stereoscopic illustration cannot be drawn independently of the other member of the pair because certain features (e.g., which octant of an ellipsoid is shaded) must be done identically in the two drawings. In ORTEP the "stereoscopically sensitive decisions" are handled by using two Cartesian coordinate systems: the reference system and the working system (see 3.1.8). The steps involved in picture composition (see 2.2.2) and the stereoscopically sensitive decisions are always based on the reference system, but the drawing of the illustration (see 2.2.3) is always based on the working system. A stereoscopic rotation is simply a rotation of the working system *from the reference system* about the axis that is vertical while viewing the final result. For example, a nominal rotation of +2.7° about the plot's *y* axis might be used for the left-eye view and a rotation of -2.7° about the same axis might be made before plotting the right-eye view, thus producing a total interocular angle of 5.4°.

### 2.3.2 Repeating a Sequence of Operations

It should be noted that steps 8 and 9 in the program to draw a stereo pair, which actually comprise several ORTEP instructions, are identical to steps 4 and 5. The program can be shortened somewhat by using the “save sequence” instructions (see 3.3.11). An 1101 instruction (start save sequence) would be placed before step 4, and an 1102 instruction (end save sequence) after 5. Then steps 8 and 9 can be replaced by a single 1103 instruction (execute save sequence).

Any sequence of instructions can be saved in this manner and repeated as many times as desired with 1103 instructions. For example, the save sequence feature can be used to produce a complete series of views of a structure at 15° intervals about an axis. Note that the instructions between the start and end instructions are *both executed and saved* the first time through.

## 2.4 DRAWING THE CUBANE STRUCTURE: AN EXAMPLE

The standard example for illustrating the use of ORTEP is the novel compound cubane ($C_8H_8$), whose structure was published by Fleischer in 1964.[5] In cubane, the carbon-carbon bonds lie along the edges of a cube within experimental error. The compound crystallizes with the trigonal symmetry of space group R$\bar{3}$. The $\bar{3}$ axis lies along a body diagonal of the molecule, and as a result the compound contains only four unique atoms. These are one carbon and its attached hydrogen in general positions off the $\bar{3}$ axis (C1 and H1) and one carbon and its hydrogen in special positions on the $\bar{3}$ axis (C2 and H2). Anisotropic temperature factor coefficients were fitted to the carbon atoms during the least-squares refinement of the structure, and isotropic temperature factors were used for the hydrogen atoms. The anisotropic temperature factors given for the carbon atoms are of the type called zero† in this report (see 3.2.4.2).

To draw the structure the following information is needed:

| | |
|---|---|
| Cell Parameters | $a = b = c = 5.34$ Å, $\alpha = \beta = \gamma = 72.26°$ |
| Equivalent Positions of Space Group R$\bar{3}$ | $x, y, z$   $z, x, y$   $y, z, x$   $\bar{x}, \bar{y}, \bar{z}$   $\bar{z}, \bar{x}, \bar{y}$   $\bar{y}, \bar{z}, \bar{x}$ |
| Positional Parameters<br>C1<br>C2<br>H1<br>H2 | *x*   *y*   *z*<br>−0.18711   0.19519   0.10706<br>0.11546   0.11546   0.11546<br>−0.32460   0.34680   0.18480<br>0.21000   0.21000   0.21000 |
| Anisotropic Temperature Factor Coefficients<br>C1<br>C2 | $b_{11}$   $b_{22}$   $b_{33}$   $b_{12}$   $b_{13}$   $b_{23}$<br>0.0410   0.0425   0.0450   −0.0042   −0.0142   −0.0051<br>0.0468   0.0468   0.0468   −0.0143   −0.0143   −0.0143 |

†Occasionally authors of structure papers neglect to define the equation for the anisotropic temperature factor coefficients. In the present case, the type can be determined from the comparative isotropic temperature factor listed in anisotropic form in Fleischer’s Table II.[5] In other instances, one must arbitrarily choose a type (usually 0, 1, or 4 in the USA), do the principal axis transformation, and then check that the principal values are correct, or at least reasonable. In particular, the principal values must all be positive.

### 2.4.1 Data Input for Cubane

#### 2.4.1.1 Title Card

The first line of input is a job title (see 3.2.1).

```
 CUBANE, E.B. FLEISCHER, J. AM. CHEM. SOC., 86, 3889 (1964)
```

#### 2.4.1.2 Cell Parameter Card

Cell parameters are provided on the second line (see 3.2.2). The "1" in the first column signals the format of the symmetry information that follows.

```
1    5.34     5.34     5.34    72.26    72.26    72.26
```

#### 2.4.1.3 Symmetry Cards

The symmetry operators of the space group begin on line 3 of the input (see 3.2.3). The last of these has a numeric value other than "0" in column 1.

```
  x, y, z
  z, x, y
  y, z, x
  -x, -y, -z
  -z, -x, -y
1 -y, -z, -x
```

#### 2.4.1.4 Atomic Parameter Cards

Two cards are required for each atom. The first gives the atom's positional parameters (see 3.2.4.1), and the second provides its thermal parameters (see 3.2.4.2). The last atom has a "1" in column 1 of its thermal parameter card. Atoms are frequently referenced in the ORTEP instructions by their numeric position within this list.

Atoms 1 and 2 are entered with positional parameter Type 0 and anisotropic temperature factor Type 0.

```
  C1                        -.18711   .19519   .10706        0
0  .04100   .04250   .04500  -.00420  -.01420  -.00510        0
  C2                         .11546   .11546   .11546        0
0  .04680   .04680   .04680  -.01430  -.01430  -.01430        0
```

Atoms 3 and 4 are entered with positional parameter Type 0 and with dummy sphere temperature factors (Type 7) with a radius of 0.1 Å before scaling.

```
  H1                        -.32460   .34680   .18480        0
0     .10                                                     7
  H2                         .21000   .21000   .21000        0
0     .10                                                     7
```

A dummy atom (atom 5) at the cell origin is also included with a blank card dummy sphere. This could also be entered with Type 7 as were atoms 3 and 4.

```
 ORGN                                  0         0         0         0
1                                                                    0
```

### 2.4.2 Analysis of Structure

The 100 series instructions (see 3.3.2) are neither associated with nor required for producing an illustration. They are shown here to demonstrate how they are used. A 101 instruction is used to obtain a tabulation of the atoms surrounding one atom or a series of several designated atoms. For example, to obtain a list of all atoms (hydrogen and carbon atoms) out to a distance of 3.61 Å about the two carbons C1 and C2, the following 101 instruction would be used.

$$\texttt{101}\quad \underbrace{\texttt{155501}\qquad\texttt{2}}_{\text{(a)}}\qquad \underbrace{\texttt{1}\qquad\texttt{4}}_{\text{(b)}}\quad \underbrace{\texttt{3.61}}_{\text{(c)}}$$

where the parts designate:

(a) origin atoms 1 through 2 of symmetry operation 1,
(b) target atoms 1 through 4 of all symmetry and translation operations, and
(c) a distance $D_{\max}$ of 3.61 Å.

A 102 instruction gives both interatomic distances and interatomic angles. The following instruction could be used to find all covalent bonds and bond angles about the two carbons.

```
102   155501         2         1         4       1.8
```

In this case a smaller $D_{\max}$ is used so that only the distances and angles of immediate interest would be computed since there are $n(n - 1)/2$ angles for $n$ interatomic vectors about an atom.

### 2.4.3 Programming the Cubane Illustration

First, plotting is initialized with a 201 instruction (see 3.3.3).

```
201
```

The two plot boundary dimensions can be equal for the present illustration since the cubane molecule is a cube. A 2.8 × 2.8 inch boundary is specified with a 0.25 inch margin to give a 2.3 × 2.3 inch square working area. A 10 inch view distance might be reasonable to use in viewing a model of this size. These are set with a 301 instruction. (See 3.3.4.1.)

```
301       2.8       2.8       10.       .25
```

The subject of the illustration is a single complete cubane molecule. Since all the atoms of the molecule were not provided in the input atoms list, the “missing” atoms may be found by using a 402 instruction to specify a sphere of enclosure, centered on the dummy atom 5, which is at the center of a cubane molecule. A radius of 3.2 Å should be adequate to find all the atoms and isolate a single molecule. The atoms found by this instruction are stored in the ATOMS array. (See 3.3.5.2.)

```
402   555501          5         1           4      3.2
      └───────────────┘         └───────────┘      └──┘
             (a)                     (b)            (c)
```

where the parts designate:

(a) a run of origin atom(s) representing sphere centers from atom 5 to atom 5 in symmetry position 55501 (in this example, a single sphere),
(b) a run of target atoms from atom 1 to atom 4, and
(c) a sphere radius of 3.2 Å.

A 501 instruction is used to establish a coordinate system for orienting the molecule. In this case, the coordinate system is defined along the edges of the cubane cube. The origin is positioned on the dummy atom 5. The desired coordinate system orientation is defined by specifying two vectors from the special position atom 255501 to the two symmetry-related general-position atoms 155501 and 155502. (See 3.3.6.1.)

```
501   555501   255501   155501   255501   155502        0        0
```

A 502 instruction is used to rotate the molecule relative to the established coordinate system to optimize the appearance of the illustration. A rotation of 25° about the *y* axis (axis 2) followed by a rotation of 28° about the *x* axis (axis 1) will produce a satisfactory view of the molecule. (See 3.3.6.2.)

```
502          2      25.          1      28.
```

To position and scale the subject for projection onto the “drawing board” and to utilize all available space, a 604 instruction is used, which automatically sets the origin and drawing scale. It also sets the ellipsoid scale factor ratio SCAL2 to the value corresponding to 50% probability unless a non-zero value is supplied on the instruction card. (See 3.3.7.1).

```
604          0          0          0          0
```

The stereoscopic rotation for the left eye is specified next with a 503 instruction. A rotation of 2.7° about the *y* axis (axis 2) is used. Later in the program, a –2.7° rotation about the same axis will be made for the right-eye view to give a total interocular angle of 5.4°. (See 3.3.6.3.)

```
503          2      2.7
```

Since the structure will be drawn twice, once for each eye, the “save sequence” feature is used to shorten the program. Note that the instructions between the start (1101) and end (1102) are *both executed and saved* the first time through. They can then be re-executed as many times as desired by using the “execute save sequence” instruction 1103. (See 3.3.11.) The 1101 instruction starts the save sequence.

```
1101
```

The 1001 (or 511) instruction stores the information needed for the overlap hidden-line correction (i.e., as a projected boundary ellipse for each atom in the ATOMS array and a quadrangle approximation for each bond). The bonds are specified with a Format No. 2 trailer card identical to that used in the 812 instruction described below. (See 3.3.12.1.)

```
2 1001
        1  4  1  4  4   0.9   1.6   .04
```

The ATOMS array currently contains all the atom designators for one cubane molecule. The molecule is drawn in two separate steps so that the hydrogen and carbon atoms can be given different graphical representations. To draw the carbon atoms (ANR = 1,2), a standard model produced with the 716 instruction (new in ORTEP-III) is used. [This model is the same as that produced with a 705/715 instruction that (a) draws the three principal-plane forward traces and the boundary-plane trace (NPLANE = 4), (b) omits the reverse sides of the principal planes (NDOT = 0), (c) draws the forward principal axes without additional shading (NLINE = 1), and (d) omits the reverse principal axes (NDASH = 0).] In addition, chemical symbols are drawn with letters 0.07 in. high (before projection) and displaced from the atomic centers by 0.18 in. horizontally and 0.21 in. vertically. (See 3.3.8.)

```
1  716                                                   .07      .18      .21
     0        0        0        1        2
```

The hydrogen atoms (ANR = 3, 4) are drawn with a different standard model (instruction 712) than the carbon atoms. Chemical symbols are 0.07 in. high and offset 0.15 in. horizontally and 0.13 in. vertically.

```
1  712                                                   .07      .15      .13
     0        0        0        3        4
```

The most convenient procedure for drawing bonds is to use the implicit bond instruction 812 (see 3.3.9.2). All other information can be entered with a single Format No. 2 trailer card.

```
2  812
     1  4  1  4  4   0.9   1.6   .04
    |_____|_____|___|___________|_____|
      (a)   (b)  (c)     (d)      (e)
```

where the parts designate:

(a) origin atom number run of those atoms that must be at one end of each bond,
(b) target atom number run of those atoms that must be at the other end of each bond,
(c) bond type 4,
(d) the distance range, 0.9 to 1.6 Å, that will cover all covalent bond distances, and
(e) the bond radius, 0.04 Å.

The remaining fields on the card are blank since a complete set of bond distance labels is not desired.

The last feature of the illustration is the labeling with 900 instructions (see 3.3.10). Because of the symmetry, there are only two different C–C bond lengths in cubane. These are C1–C1 and C1–C2. One example of each of these bonds is labeled. For variety, one is labeled with a normal bond-length label and the other with a perspective label. The two bonds that can be labeled most advantageously are 155504–155503 and 255504–155505. The labels will be 0.07 in. high and displaced vertically from the bond center by -0.2 in.

```
     906   155504   155503         0         0      .07         0       -.2
     916   255504   155505         0         0      .07         0       -.2
```

Finally, a caption for the illustration is drawn. This can conveniently be positioned by “hanging” it from the dummy atom 555501 and “bouncing” it 1.8 in. from the left *x* boundary and 0.3 in. from the lower *y* boundary. The caption is 0.15 in. high.

```
  3  902   555501         0       1.8       0.3      .15         0         0
CUBANE
```

The save sequence is now terminated.

```
    1102
```

The plotting origin is then shifted 2.375 in. along *x* with a 202 instruction in preparation for the right-eye view.

```
     202    2.375
```

The stereo rotation of -2.7° about axis 2 is now performed for the right-eye view with a 503 instruction. (Note that this rotation starts with the reference orientation, not the previous working orientation.)

```
     503         2     -2.7
```

The save sequence is now repeated for the right eye. (Note that the ATOMS array contains the same information that it did when the first view was drawn.)

```
    1103
```

The illustration is now complete. Plotting is terminated with a 202 instruction with no parameters.

```
     202
```

Finally, a -1 instruction terminates the program. (See 3.3.13.)

```
      -1
```

### 2.4.4 Illustration of the Example

Figure 2.1 shows a stereoscopic illustration of cubane exactly as it was produced by ORTEP. The drawing has not been retouched. Note that one bond distance label was drawn in perspective along the bond, and the other was drawn as a regular label parallel to the page.

Note , too, that while most of the atom labels are easy to read and it is clear which atoms they are labeling, some are in locations where the atom being labeled is ambiguous and some are not corrected for overlap. The first problem is the result of labeling a number of atoms with the 700 instruction that draws the atoms. More precise placement can be accomplished by labeling atoms individually (see 7.1) though this can be a time consuming process.

Overlap, particularly for chemical symbols and bond distance labels, is often one of the major problems encountered when producing an illustration. For nonstereoscopic figures, it may be better to add the lettering after the drawing is completed. However, for stereoscopic figures, adding the lettering after the illustration is produced is unsatisfactory because of the necessity for exact relative placement of the lettering on the two views to maintain good stereopsis. In this case, it is best to let ORTEP place the lettering.

The ORTEP input consisting of the crystal data and ORTEP instructions used to produce the structure illustration immediately follows the figure. The example utilizes a wide range of instructions in order to demonstrate their use. As is the case with any programming system, there are many ways of doing a given problem. The user should examine the example carefully since several useful techniques are illustrated. Additional examples are provided in Section 7.

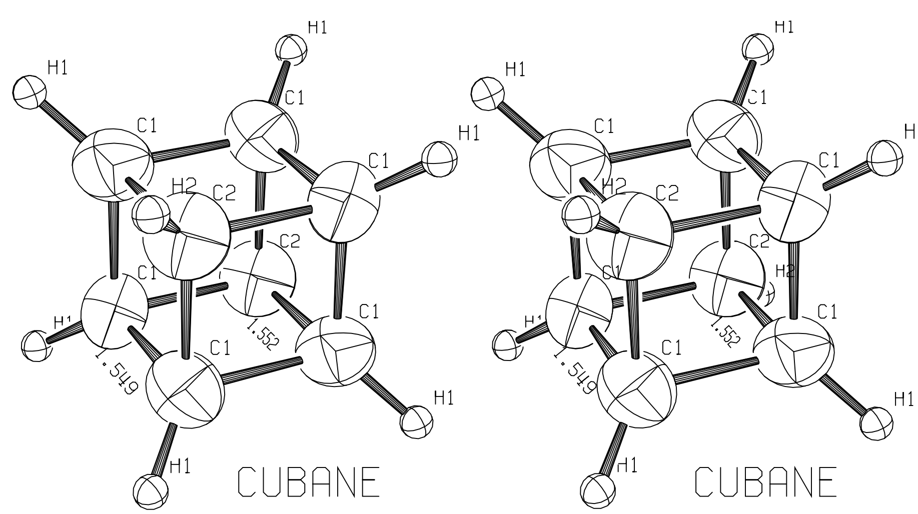


**Fig. 2.1. Cubane drawn by ORTEP as a stereoscopic pair.**

```
 CUBANE, E.B. FLEISCHER, J. AM. CHEM. SOC., 86, 3889 (1964)
1    5.34     5.34     5.34    72.26    72.26    72.26
  x, y, z
  z, x, y
  y, z, x
  -x, -y, -z
  -z, -x, -y
1 -y, -z, -x
  C1                       -.18711   .19519   .10706        0
   .04100   .04250   .04500  -.00420  -.01420  -.00510        0
  C2                        .11546   .11546   .11546        0
   .04680   .04680   .04680  -.01430  -.01430  -.01430        0
  H1                       -.32460   .34680   .18480        0
      .10                                                   7
  H2                        .21000   .21000   .21000        0
      .10                                                   7
 ORGN                            0        0        0        0
1                                                           0
# FIND ALL NEIGHBOR ATOMS AROUND C1 AND C2 OUT TO 3.61 A
      101   155501        2        1        4     3.61
# FIND COVALENT BONDS AND BOND ANGLES AROUND CARBONS
      102   155501        2        1        4      1.8
# INITIALIZE PLOTTING
      201
# 2.8x2.8 BOUNDARY, 2.3x2.3 INSIDE 0.25 MARGIN, VIEW FROM 10 INCHES
      301      2.8      2.8      10.      .25
# ENCLOSER SPHERE OF RADIUS 3.2 A ABOUT DUMMY ATOM 5,555,01
      402   555501        5        1        4      3.2
# ORIGIN ON DUMMY ATOM 555501, VECTORS ALONG 2 EDGES OF CUBANE
      501   555501   255501   155501   255501   155502                 0
# ROTATE 25 DEGREES ABOUT Y, THEN 28 DEGREES ABOUT NEW X
      502        2      25.        1      28.
# AUTOMATIC SCALE AND POSITION, 50 PERCENT PROBABILITY ELLIPSOIDS
      604        0        0        0        0
# STEREO ROTATION OF 2.7 DEGREES ABOUT Y FOR LEFT EYE
      503        2      2.7
# START SAVE SEQUENCE
     1101
# STORE PROJECTED ATOMS AND BONDS FOR OVERLAP, MARGIN SET BY DEFAULT
  2  1001        0
           1  4  1  4  4   0.9   1.6   .04
# DRAW CARBON ATOM ELLIPSOIDS, ATOM NUMBER RUN 1-2
  1   716                                         .07      .18      .21
                                 1        2
# DRAW HYDROGEN ATOM SPHERES, ATOM NUMBER RUN 3-4
  1   712                                         .07      .15      .13
                                 3        4
# TYPE 4 BONDS .04 A MEAN RADIUS, ATOMS 1-4 TO ATOMS 1-4, 0.9-1.6 A
  2   812
           1  4  1  4  4   0.9   1.6   .04
# LABEL BOND 155504-155503 WITH REGULAR BOND DISTANCE LABEL
      906   155504   155503        0        0      .07        0      -.2
# LABEL BOND 255504-155505 WITH PERSPECTIVE BOND DISTANCE LABEL
      916   255504   155505        0        0      .07        0      -.2
```

```
# DRAW TITLE
  3   902   555501         0       1.8       0.3       .15         0         0
CUBANE
# END SAVE SEQUENCE
     1102
# SHIFT DRAWING ORIGIN 2.375 INCHES ALONG X
      202    2.375
# STEREO ROTATION OF -2.7 DEGREES ABOUT Y FOR RIGHT EYE VIEW
      503         2     -2.7
# EXECUTE SAVE SEQUENCE FOR RIGHT EYE DRAWING
     1103
# TERMINATE PLOTTING
      202
# TERMINATE ORTEP
       -1
```