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DECUS NO.	8-293
TITLE	ATOMIC COORDINATE PROGRAM
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SOURCE LANGUAGE	MACRO 8

Coordinate Program*

This program consists of a main program and a large number of subroutines which are designed to facilitate developing the coordinates of the atoms of a given molecule. Loading information is allowed by a description of the available options, and of the algorithms which are used. The program occupies essentially all of core except for that used by version C of the floating point interpreter. Some locations normally used by the interpreter are also used, so that it is necessary to load the interpreter before loading the program. The binary tape which is supplied contains both the interpreter and the program.

Loading

The binary tape is loaded in the usual fashion via the binary loader. The starting address is 200. In case of an error, recovery can be made by restarting at 4746 or 1026. If this does not work, reload the program (this does not erase data) and restart at one of these locations.

Operation and Options

On starting, the computer will type

```
ATOM 1 IS AT 0, 0, 0
ATOM 2,  R(1, 2) =
```

The 1-2 bond length is then typed followed by a space. The computer now types

```
ATOM 3,  R(2, 3) =
```

---

* The development of this program was assisted by a National Science Foundation Grant.

The bond length is typed followed by a space. The response is ANGLE (1, 2, 3)=. The bond angle is typed. Atoms 1, 2 and 3 are placed in the x, y plane, with atom 2 lying on the x axis. Further atoms require information on bond length, bond angle and torsional angles. Thus, the computer types

NOW TYPE R(K, L), ANGLE(J, K, L) and TORS (I, J, K, L) WHERE L IS THE NEW ATOM
I J K L R(K, L) ANGLE TORS

Integer values for the indices are now typed followed by decimal values for the bond length, angle and torsional angle. Each value is followed by a space. As an example, for cyclohexane with tetrahedral angles, the initial values of R(1, 2)=1.54, R(2, 3)=1.54 and ANGLE(1, 2, 3)=109.5 would be followed by

```
01 02 03 04 1.54 109.5  60.0
02 03 04 05 1.54 109.5 -60.0
03 04 05 06 1.54 109.5  60.0
```

The coordinates of the carbons will now have been developed. An exit from this mode of operation is effected by giving the first index a value of -1. The computer then types > and waits for the control letter followed by a space. The set of control letters and their effect is given in Table I.

As a check on the coordinates defined by the values given above (note that one torsional angle must be negative in order to close the ring), we may type $R^{b}1^{b}6^{b}$. (The superscript b indicates a space). The computer then answers with 1.54 indicating the correct distance. One bond has not been defined by the data given above - that between atoms 1 and 6. This information is needed if the coordinates are to be plotted later. To add this type E, followed by a space. The computer responds with

```
ATOMS
00010002
00020003
00030004
00040005
00050006
ADD
```

Now, type $1^{b}6^{b}$ to insert the additional bond. Terminate mode by typing -1 followed by a blank. The computer responds with DELETE. Since no pair of atoms is to be deleted, respond with -1 followed by a blank. The computer now types > and waits for another command.

The secondary hydrogens may now be added. The sequence would be

```
S 6 1 2 1.1 106.0
S 1 2 3 1.1 106.0
S 2 3 4 1.1 106.0
S 3 4 5 1.1 106.0
S 4 5 6 1.1 106.0
S 5 6 1 1.1 106.0
```

Here, S indicates that two hydrogens are to be added to the second atom of the list that follows (cf Table I). The three numbers give the indices of the atoms forming the C-C-C bond to which the hydrogens are to be added. The next number gives the bond length and is followed by the H-C-H bond angle.

The secondary hydrogens will now have been added using the specified bond length and angle. The set of coordinates which have been developed may be outputted by typing $P^{b}0^{b}$(zero). If the coordinates are to be punched on tape for later tape to card conversion, type $P^{b}\text{-}1^{b}$. The computer halts, and the punch may be turned on. Pressing CONTINUE will cause the coordinates to be printed and punched in decimal form, and the computer again halts. If the tape is to be loaded back into the computer at a later time, shut off punch, put teletype on local, turn on punch and type 00^{b}. In either case, the program is continued by pressing CONTINUE.

The other options should be fairly clear from the descriptions in Table I. The one designated by L is particularly useful. If one wishes to replace a hydrogen with a methyl group, for example, one may translate so that the coordinates of the carbon to which it is attached is 0, 0, 0. Then L followed by the coordinates of the hydrogen will rotate the entire set of coordinates so that the hydrogen will lie on the z axis. Using the change (C) option, the hydrogen may be replaced by a carbon with the appropriate C-C bond length. The coordinates of methyl hydrogens may be added by translating to make the coordinates of the new carbon 0, 0, 0 and adding the following using the fix (F) option:

```
01 0.0 -1.0343 0.374
02 0.8957 0.5172 0.374
03 -0.8957 0.5172 0.374
00
```

Note that a zero followed by a number and a blank must precede each set of floating point numbers. This is necessary so that the computer may ignore leader, line feed and carriage return characters when a tape is read in using the F option. The computer initially checks each character to see if it is a zero. When it finds the first zero, it reads the <u>following</u> number. If the number is greater than zero, the x, y and z coordinates are read using the floating point interpreter. If the number is zero, an exit from the subroutine is called and another option character is requested. If a particular orientation of the methyl group with respect to the rest of the molecule is desired, the molecule may be suitably rotated about the z axis ($U^{b}3^{b}v$ where v is the number of degress) before adding the hydrogen coordinates.

The program will accept up to 42 atoms. A larger number will result in destroying data and part of the program. No check is provided to guard against this possibility. Particular attention should be paid to the bond register. If a large number of changes in coordinates are made, it is possible for this register to overflow without exceeding 42 atoms. It should therefore be checked occasionally - and it will have to be correct if the WRITE program is to operate correctly. In deleting coordinates using the delete (D) option, it is important to note that an attempted deletion of non-existent data (i. e. $n_1 >$ no. of atoms) results in deleting the coordinates of the last atom in the list.

It is possible to have difficulty entering hydrogens using the S option for certain arrangements of atoms. This is not a frequent occurrence and may be corrected by deleting the incorrect atoms. rotating the coordinates and using S again. The bond register also will have to be corrected.

The WRITE (on CRT) option is described in a separate writeup.

A sample run using this program is appended.

```
CYCLOHEXANE
```
← typed on "local" before starting program

```
CALCULATE ATOMIC COORDINATES
```
← initial program typeout

```
ATOM 1 IS AT 0,0,0
ATOM 2, R(1,2) =1.54
ATOM 3, R(2,3) =1.54  ANGLE (1,2,3) =109.5
NOW TYPE R(K,L), ANGLE(J,K,L) AND TORS(I,J,K,L) WHERE L IS
THE NEW ATOM
```
} 1st three atoms are defined

```
 I  J  K  L R(K,L) ANGLE TORS
01 02 03 04 1.54 109.5 60.0
02 03 04 05 1.54 109.5 -60.0
03 04 05 06 1.54 109.5 60.0
-1
>R 1 6 +0.1542879E+01
```
} here, the carbon skeleton is built up

R asks for bond length (undefined bond is checked)

```
>A 2 1 6 +0.1094618E+03
```
A asks for bond angle (undefined angle is checked)

```
>E
```
← E asks for listing of bond register

```
ATOMS
00010002
00020003
00030004
00040005
00050006
```
} atoms which are bonded, ie. 1-2, 2-3 etc.

```
ADD 1 6
```
add the 1,6 bond

```
ADD -1
```
-1 terminates mode

```
DELETE -1
```
-1 terminates mode.

```
>S 6 1 2 1.1 106
>S 1 2 3 1.1 106
>S 2 3 4 1.1 106
>S 3 4 5 1.1 106
>S 4 5 6 1.1 106
>S 5 6 1 1.1 106
```
} S puts in secondary hydrogens on middle atom of list, with 1.1 Å bond lengths and 166° bond angles

```
>P 0
```
← P asks for printout. 0 gives all coordinates in floating point form, a number gives just that coordinate, and -1 gives a different format printout following a HALT (press CONT) to allow punch to be turned on

```
ATOM          X                Y                Z
0001  +0.0000000E+00  +0.0000000E+00  +0.0000000E+00
0002  +0.1539999E+01  +0.0000000E+00  +0.0000000E+00
0003  +0.2054054E+01  +0.1451670E+01  +0.0000000E+00
0004  +0.1541440E+01  +0.2178525E+01  -0.1257180E+01
0005  +0.1441717E-02  +0.2180052E+01  -0.1258062E+01
0006  -0.5140514E+00  +0.7288928E+00  -0.1258945E+01
0007  -0.3815353E+00  +0.4892026E+00  +0.9083559E+00
0008  -0.3815352E+00  -0.1031332E+01  +0.2801060E-01
0009  +0.1922070E+01  -0.5406136E+00  +0.8784978E+00
0010  +0.1922070E+01  -0.5406136E+00  -0.8784978E+00
0011  +0.1719231E+01  +0.1975553E+01  +0.9074350E+00
0012  +0.3153556E+01  +0.1467640E+01  +0.2893292E-01
0013  +0.1924548E+01  +0.3209266E+01  -0.1285477E+01
0014  +0.1923544E+01  +0.1688022E+01  -0.2164595E+01
0015  -0.3805962E+00  +0.2720688E+01  -0.3795649E+00
0016  -0.3795888E+00  +0.2721399E+01  -0.2136560E+01
0017  -0.1613584E+01  +0.7146030E+00  -0.1287592E+01
0018  -0.1802634E+00  +0.2059813E+00  -0.2167322E+01
```

```
>
```
Another command is requested

Table I

Control Characters and Their Effect*

Character and List	Effect
R n_1 n_2	The distance between atoms n_1 and n_2 is typed.
A n_1 n_2 n_3	The angle formed by atoms n_1, n_2 and n_3 is typed.
T n_1 n_2 n_3 n_4	The torsional angles formed by atoms n_1, n_2, n_3 and n_4 is typed.
S n_1 n_2 n_3 v_1 v_2	Secondary hydrogens are added to atom n_2 which is attached to n_1 and n_3. The bond length is v_1 and the HCH bond angle is v_2.
M n_1 n_2 n_3 n_4 v_1	A methine hydrogen is added to atom n_1 which is attached to atoms n_2, n_3 and n_4. The bond length is v_1.
G	Get additional coordinates. A new set of indices, bond length, bond angle and torsional angle is then typed. Exit from this mode is made by typing -1 as before.
C n_1 v_1 v_2 v_3	Change the coordinates of atom n_1 to v_1, v_2, v_3.
D n_1	Delete the coordinates of atom n_1. If n_1 is greater than the number of atoms, the coordinates of the last atom are deleted.
I n_1 v_1 v_2 v_3	Insert the coordinates v_1, v_2, v_3 before those of atom n_1.
F n_1 v_1 v_2 v_3	Fix the coordinates of another atom as v_1, v_2, v_3. Additional coordinates may be added until a zero value of n_1 is reached. The computer then asks for a new instruction. n_1 must be preceded by a zero in each case. Thus, the last entry is 00 followed by a space.
E	Examine bond registers. The attached atoms are listed in pairs. The computer then types ADD. Additional bonding pairs may now be entered. Adding is terminated by -1. The computer then types DELETE. The number in the list of the entry to be deleted may now be typed. This mode is terminated by -1.

P n_1	Print coordinates. If n_1 is zero, all coordinates are typed in floating point form. If n_1 is positive, the coordinates of atom n_1 are typed. If n_1 is negative, the computer halts, permitting the punch to be turned on. Pressing the CONTINUE key leads to typing of coordinate values in decimal form. The computer again halts and is restarted by pressing the CONTINUE key. If the tape is to be read back into the computer at a later time, terminate the tape with 00 (see text).
W	Write coordinates in CRT. This leads to the message "LOAD SECOND TAPE, START AT 4400." See writeup of the WRITE subroutine.
B n_1	Invert the values of the $x(n_1=1)$, $y(n_1=2)$ or $z(n_1=3)$ array (i. e. multiply them by -1. 0).
L v_1 v_2 v_3	Rotate the vector defined by v_1, v_2, v_3 so that it lies along the z axis.
Q n_1 n_2	Transpose arrays n_1 and n_2 (i. e. exchange them). For x, n=1; y, n=2; z, n=3.
U n_1 v_1	Rotate about axis n_1 by v_1 degrees.
V n_1 v_1 v_2 v_3	If n_1 is a positive integer, translate coordinates of atom n to 0, 0, 0- ignore v_1, v_2, v_3. If n_1 is zero or negative, translate coordinates to make v_1, v_2, v_3=0, 0, 0.

*The values designated as n are integers, those designated by v are decimal numbers. A space or carriage return must follow each entry.

If the control character is entered incorrectly, type it a second time. The computer will respond with a "?", followed by > . Then a new character may be entered.

If an integer is entered incorrectly, type a back arrow (←) before the terminating space. Then type the entire correct number. If the space is typed, stop computer and restart at 4746.

If a decimal (floating point) number is entered incorrectly, type a "rubout" before the terminating space. Then type the entire correct number.

Method of Calculation

The first atom is located at 0, 0, 0 and its bond to the second atom is considered to lie on the x axis. The third atom is placed in the xy plane with $x_3 = x_2 - r_{23}\cos\theta$ and $y_3 = \sin\theta$.

The remaining atoms are located as follows where R is the bond length between atoms k and l, θ is the bond angle formed by atoms j, k and l, and ϕ is the torsional angle formed by atoms i, j, k and l. A new coordinate system is set up so that

$$x_l' = R\cos\theta$$

$$y_l' = R\sin\theta\cos\phi$$

$$z_l' = R\sin\theta\sin\phi$$

Then the transformation matrix is obtained which will transform the new coordinate system into the original system. Thus:

$$x_l = x_k + T_{xx}\cdot x_l' + T_{xy}\cdot y_l' + T_{xz}\cdot z_l'$$

$$y_l = y_k + T_{yx}\cdot x_l' + T_{yy}\cdot y_l' + T_{yz}\cdot z_l'$$

$$z_l = z_k + T_{zx}\cdot x_l' + T_{zy}\cdot y_l' + T_{zz}\cdot z_l'$$

The transformation matrix is obtained as follows:

$$R_{ab} = \sqrt{(x_j-x_k)^2 + (y_j-y_k)^2 + (z_j-z_k)^2}$$

$$T_{xx} = (x_j-x_k)/R_{ab} \qquad T_{yx} = (y_j-y_k)/R_{ab} \qquad T_{zx} = (z_j-z_k)/R_{ab}$$

$$SCALE = (x_i-x_k)T_{xx} + (y_i-y_k)T_{yx} + (z_i-z_k)T_{zx}$$

$$R_1 = (x_i-x_k) - SCALE\cdot T_{xx}$$

$$R_2 = (y_i-y_k) - SCALE\cdot T_{yx}$$

$$R_3 = (z_i-z_k) - SCALE\cdot T_{zx}$$

$$RAJ = \sqrt{R_1^2 + R_2^2 + R_3^2}$$

$$T_{xy} = R_1 / RAJ \qquad T_{yy} = R_2 / RAJ \qquad T_{zy} = R_3 / RAJ$$

$$T_{xz} = T_{yz} \cdot T_{zy} - T_{zx} \cdot T_{yy}$$

$$T_{yz} = T_{zx} \cdot T_{xy} - T_{xx} \cdot T_{zy}$$

$$T_{zz} = T_{xx} \cdot T_{yy} - T_{yx} \cdot T_{xy}$$

The bond lengths and bond angles are calculated using the usual relationships. The dihedral angle (ϕ) is calculated as follows where atoms 1, 2, 3and 4 define the angle:

$$C = [(y_1 - y_2)(z_2 - z_3) - (z_1 - z_2)(y_2 - y_3)] \cdot [(y_4 - y_3)(z_2 - z_3) - (z_4 - z_3)(y_2 - y_3)]$$
$$+ [(z_1 - z_2)(x_2 - x_3) - (x_1 - x_2)(z_2 - z_3)] \cdot [(z_4 - z_3)(x_2 - x_3) - (x_4 - x_3)(z_2 - z_3)]$$
$$+ [(x_1 - x_2)(y_2 - y_3) - (y_1 - y_2)(x_2 - x_3)] \cdot [(x_4 - x_3)(y_2 - y_3) - (y_4 - y_3)(x_2 - x_3)]$$

$$D = \{[(y_1 - y_2)(z_2 - z_3) - (z_1 - z_2)(y_2 - y_3)]^2 + [(z_1 - z_2)(x_2 - x_3) - (x_1 - x_2)(z_2 - z_3)]^2$$
$$+ [(x_1 - x_2)(y_2 - y_3) - (y_1 - y_2)(x_2 - x_3)]^2\}^{\frac{1}{2}} \cdot \{[(y_4 - y_3)(z_2 - z_3) - (z_4 - z_3)(y_2 - y_3)]^2$$
$$+ [(z_4 - z_3)(x_2 - x_3) - (x_4 - x_3)(z_2 - z_3)]^2 + [(x_4 - x_3)(y_2 - y_3) - (y_4 - y_3)(x_2 - x_3)]^2\}^{\frac{1}{2}}$$

$$\phi = \cos^{-1}(C/D)$$

Coordinate Program Storage Map

0002-0037 0063-0177	Page 0 constants	
0200-1023	Initial operating program	
1025-1177	PRNT-	Subroutine control program
1200-1265	ANGLES-	Bond angle subroutine
1266-1277	RVAL-	Bond distance subroutine
1300-1327	SDIST-	Subroutine for calculating distance between points
1330-1372	TRPOSE-	Subroutine for transposing coordinates
1373-1457	DELETE-	Subroutine for deleting coordinates
1460-1562	ROT2-	Subroutine for rotating about an axis
1563-1633	TRANSL-	Subroutine for translating coordinates
1634-1732	LOCATN-	Subroutine for obtaining addresses of elements in x, y and z arrays
1733-1747	CHANGE-	Subroutine for changing a coordinate
1750-1777	FIX-	Subroutine for fixing additional coordinates
2000-2060	PRINTT-	Subroutine for printing coordinates using E format
2061-2357	SECOND-	Subroutine for adding secondary hydrogens
2360-2574	TORSS-	Torsional angle subroutine
2600-2641	LIST-	Subroutine which prints coordinates - used with PRINTT
2642-2674	ARCOS-	ARC COSINE subroutine
2675-2777 4400-4520	ROT1-	Subroutine for rotating a point onto the Z axis
4521-4606	INSERT-	Subroutine for inserting a coordinate
4607-4722	TERT-	Subroutine for introducing tertiary hydrogens
4723-4745	WRITE-	Dummy write subroutine (see text)
4746-4750	RECOVR-	Error recovery subroutine
4315-4376 4143-4176	EXAMINE	Subroutine for examining bond register
3654-3703	INVERT-	Subroutine for changing sign along one coordinate
3704-3777	PRNT2-	Print selection subroutine
5000-5123 5252-5376	DCOUT-	Decimal output subroutine
5544-5562	SIGN-	Subroutine used by ROT1
4751-4756	ERR-	Subroutine used by DCOUT
3000-3177	X Array	
3200-3377	Y Array	
3400-3577	Z Array	
3600-3652	Bond register	
4000-4057	MESAGE-	Typeout subroutine (DIGITAL-8-18)
4075-4142	DECPRT-	Decimal print subroutine (DIGITAL-8-22)
4200-4311	SICONV-	Decimal input subroutine (DIGITAL-8-28)
4757-7577	Floating point interpreter "C" (with overlays from some of the above subroutines)	

```
                /PROGRAM FOR OBTAINING CARTESIAN COORDINATES
                CALL=4400
                RETURN=5400
                FSQRT=2
                FCOS=4
                FSIN=3
                FATAN=5
                BAX=146
                BAY=151
                BAZ=154
                TZ1=65
                TZ2=157
                TZ3=143
                INPUT=13
                OUTPUT=14
                FLPT=4407
                *2
0002  3000  LOCX,      3000
0003  3200  LOCY,      3200
0004  3400  LOCZ,      3400
0005  3600  LOCR,      3600
0006  0000  NN,        0
0007  5600              5600
0010  0000  LX,        0
0011  0000  LY,        0
0012  0000  LZ,        0
0013  0000  IX,        0
0014  0000  IY,        0
0015  0000  IZ,        0
0016  0000  JX,        0
0017  0000  JY,        0
0020  0000  JZ,        0
0021  0000  KX,        0
0022  0000  KY,        0
0023  0000  KZ,        0
0024  0000  IR,        0
0025  0000  ZERO,      FLTG 0.0
0026  0000
0027  0000
0030  0000  R,         FLTG 0.0
0031  0000
0032  0000
0033  7773  CONST,     FLTG 0.01745329
0034  2167
0035  6416
```

```
0036  4000  MESAGE,   4000
0037  0000  N,        0
            *63
0063  0000  INDEX,    0
0064  0003  THREE,    3
0065  0000  ANGLE,    FLTG 0.0
0066  0000
0067  0000
0070  0000  TORS,     FLTG 0.0
0071  0000
0072  0000
0073  0000  TEMP,     FLTG 0.0
0074  0000
0075  0000
0076  0000  II,       0
0077  0000  J,        0
0100  0000  K,        0
0101  0000  L,        0
0102  4200  SICONV,   4200
0103  4075  DECPRT,   4075
0104  0000  FLAG,     0
0105  0000  TX1,      FLTG 0.0
0106  0000
0107  0000
0110  0000  TX2,      FLTG 0.0
0111  0000
0112  0000
0113  0000  TX3,      FLTG 0.0
0114  0000
0115  0000
0116  0000  TY1,      FLTG 0.0
0117  0000
0120  0000
0121  0000  TY2,      FLTG 0.0
0122  0000
0123  0000
0124  0000  TY3,      FLTG 0.0
0125  0000
0126  0000
0127  0000  SS,       FLTG 0.0
0130  0000
0131  0000
0132  0000  CS,       FLTG 0.0
0133  0000
0134  0000
0135  0000  C2,       FLTG 0.0
0136  0000
0137  0000
0140  0000  RAJ,      FLTG 0.0
0141  0000
0142  0000
0143  0000  RAB,      FLTG 0.0
0144  0000
0145  0000
```

```
0146  0000  JAX,      FLTG 0.0
0147  0000
0150  0000
0151  0000  JAY,      FLTG 0.0
0152  0000
0153  0000
0154  0000  JAZ,      FLTG 0.0
0155  0000
0156  0000
0157  0000  SCALE,    FLTG 0.0
0160  0000
0161  0000
0162  0000  SUM,      FLTG 0.0
0163  0000
0164  0000
0165  0000  CAX,      FLTG 0.0
0166  0000
0167  0000
0170  0000  CAY,      FLTG 0.0
0171  0000
0172  0000
0173  0000  CAZ,      FLTG 0.0
0174  0000
0175  0000
0176  0513  CONT,     COORD
0177  1025  PRINT,    PRNT
            *3600
3600  0102            0102
3601  0203            0203
```