A NOTE ON STEREODIAGRAMS OF MOLECULES*

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ABSTRACT

The paper elucidates a simple way of deriving the coordinates for drawing stereodiagrams of molecules. This method is an alternative, but not a substitute, to the ORTEP (suggested by C. K. Johnson) which is extensively used in the literature. Illustrations are given using a program which was written based on the method mentioned here. The program is also given in an appendix for practical help.

Keywords: Stereodiagrams; perspective vision.

1. INTRODUCTION

The chemical activity of a molecule depends, apart from other factors such as charge distribution on various atoms, upon its three-dimensional structure. Knowledge of this spatial distribution of atoms in a molecule is obtained by certain physico-chemical methods, one of the accurate approaches being the x-ray crystallographic technique. Together with the three-dimensional structure so obtained, it would be of added interest and an aid to the imagination of a stereochemist to get a perspective vision of the molecule in two dimensions. Though the thermal ellipsoid program of Johnson [1] is widely used by crystallographers, for want of sufficient computer memory, and for reasons of the enormous amount of time a plotter would take, we had written a simpler program (*see* appendix), to draw perspective, but skeletal diagrams of molecules. This is achieved by obtaining the appropriate coordinates of the atoms from the input data using the imagination of an architectural engineer [2]. The input data could be the atomic coordinates in a Cartesian frame of reference or in a cylindrical polar reference system or fractions of the unit cell as generally reported in crystallographic studies. They could also be the internal parameters of the molecule such as the bond lengths, bond angles and dihedral angles from which the Cartesian coordinates of the atoms could be generated.

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2. THEORY

Due to the finite distance of separation between the eyes, the details of a 3-dimensional object seen by the right eye are different from those seen by the left. If two pictures as seen by the two eyes are printed with proper separation between them (corresponding to the separation of the eyes) and if the viewer focusses his attention at infinity, each eye sees its corresponding picture and these get " superimposed " in imagination to give a three-dimensional feeling of the object. The method adopted by Johnson to achieve this result is different from what the present author has used.

According to Johnson's program [3], a model of the molecule of suitable size is imagined at a convenient distance of say 28″ from the imaginary viewer. However this distance is adjustable. Then the model is given an additional rotation of about 2·5° to 3°, about a vertical axis, to simulate the difference between a central view and a left-eye view. The projection of the model is drawn by an incremental plotter. After completing this drawing the paper is advanced on the plotter and, after another appropriate rotation of the model, the right-eye view is drawn. It might be then reduced photographically.

The principle of the method used by the author is given below. Consider a picture plane (Fig. 1) at a distance ξ from the on-looker P (station point). Let this plane be the XY-plane of a right handed Cartesian coordinate system, the z-direction pointing towards the on-looker, and the x-axis being parallel to the line joining the two eyes. The molecular model of suitable size is

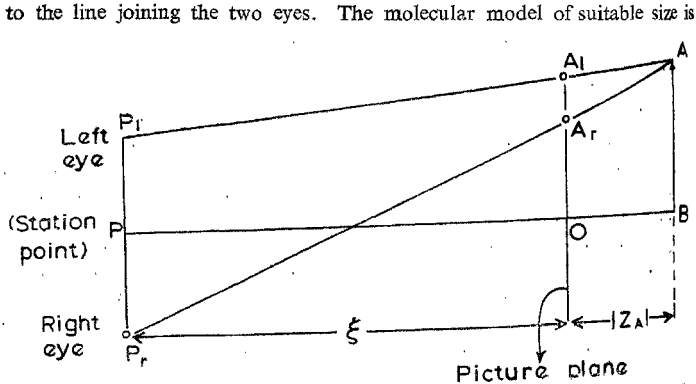

FIG. 1. Principle of getting the coordinates for stereodiagrams of molecules (using the imagination of an architectural engineer).

imagined to be behind the picture plane. Consider an Atom A. The coordinates of this atom for perspective drawing, as seen by the left and the right eye, correspond to those of A_l and A_r respectively. The lines P_lP_r, A_lO and AB are parallel to each other. Hence

$$\frac{P_lA_l}{A_lA} = \frac{P_rA_r}{A_rA} = \frac{PO}{OB} = \frac{\xi}{|z_A|}$$

Let $PP_l = PP_r = \epsilon$. Since we know the coordinates for P_l, P_r and A, we can calculate the coordinates of A_l and A_r. Thus,

$$x = \frac{\xi x_A \pm |z_A| \cdot \epsilon}{\xi + |z_A|} \tag{i}$$

$$y = \frac{\xi y_A}{\xi + |z_A|} \tag{ii}$$

$$z = 0 \tag{iii}$$

where the positive sign in the numerator of (i) is applicable for the right eye picture. A value of 72·0 cm and 3·5 cm for ξ and ϵ respectively have been found convenient. In case the diagrams are huge and overlap, they could be drawn at suitable separation and then photographically reduced to a convenient separation of about 6 to 7 cm between corresponding atoms. Alternatively, the images corresponding to the left and the right eye could be drawn with different colours (say red and blue) with a common origin. When this pair is viewed by a pair of transparent papers of the corresponding colours, the diagrams again seem to superpose in the imagination to give the stereoview [4].

3. Results

By way of example, we have shown in Fig. 2, the α-helical conformation of the backbone of a polypeptide chain [5]. The input data for this diagram were the cylindrical polar coordinates of the atoms. While it may be difficult to see from the individual diagrams of the couple, whether the chain is in the right-handed or left-handed conformation, the stereovision clearly shows that this representation is in the right-handed helical conformation. Figure 3 gives the perspective view of a cyclic dipeptide, cyclo (L-pro-D-phe) [6]. The input data for this diagram were the fractional coordinates of the atoms taken from the literature cited. It might be seen from this stereodiagram that the phenyl ring of the side chain is stacking over the 2, 5-

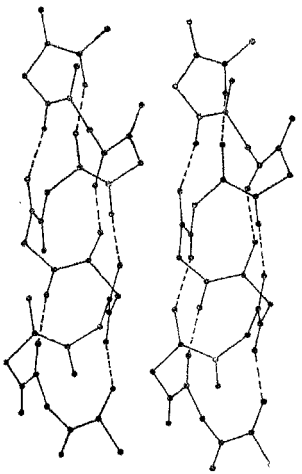

FIG. 2. Stereo pair of a fragment of polypeptide (back-bone) in the α-helical conformation.

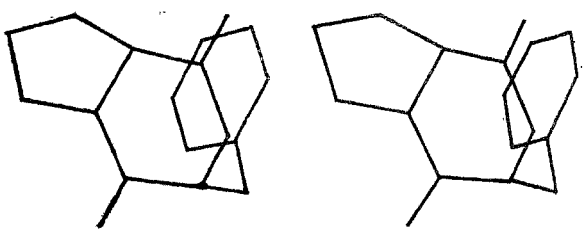

FIG. 3. Stereo pair of the molecule cyclo (D-Phe-L-Pro), showing the folded conformation.

diketopiperazine ring, which seems to be a common feature in many cyclic dipeptides [7].

4. ACKNOWLEDGEMENTS

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C       ORGAP IS FOR ORTHOGRAPHIC AND PERSPECTIVE DRAWING                  0004
        DIMENSION ANAME (100), XR (3, 100)                                 0001
        DIMENSION ATOM (3), DC (3), AMAT (3, 3), X1 (3, 1), P (3), NROT (3), PHI (3)  0002
        COMMON A, B, C, ALFA, BETA, GAMMA, NMAX, X (3, 100)                0003
        CONEA = 0·01745329                                                 0005
        READ (5, 2) NSET                                                   0006
        WRITE (6, 2) NSET                                                  0007
    2   FORMAT (20I4)                                                      0008
        DO 999 NRAM = 1, NSET                                              0009
        READ (5, 1)                                                        0010
        WRITE (6, 332)                                                     0011
        WRITE (6, 1)                                                       0012
        WRITE (6, 332)                                                     0013
    1   FORMAT (55 H.)                                                     0014
  332   FORMAT (//)                                                        0015
        READ (5, 2) NMAX, NRDCN, NTYPE, NVIEW                              0016
        WRITE (6, 2) NMAX, NRDCN, NTYPE, NVIEW                             0017
C       NMAX = MAXIMUM NO. OF ATOMS, NVIEW = NO. OF VIEW OF THE MOLECULE   0018
C       NRDCN = 1 FOR FRACTIONAL, = 2 FOR CARTECIAN, = 3 FOR CYLINDRICAL POLAR  0019
C       NTYPE = 1 FOR ORTHOGRAPHIC AND = 2 FOR PERSPECTIVE PROJECTION      0020
        READ (5, 4) ZSP, EYE                                               0021
        WRITE (6, 4) ZSP, EYE                                              0022
C       ZSP = 72·0 CM, EYE = 3·5 CM.                                       0023
    4   FORMAT (10F8·3)                                                    0024
        READ (5,3) (ANAME (I), (X (J, I), J = 1, 3), I = 1, NMAX)          0025
    3   FORMAT (A4, 3F8·4)                                                 0026
        WRITE (6, 332)                                                     0027
        WRITE (6, 333)                                                     0028
  333   FORMAT (2X, ' COORDINATES ORIGINALLY GIVEN ')                      0029
        WRITE (6, 332)                                                     0030
        WRITE (6, 31) (ANAME (I), (X (J, I), (J = 1, 3), I = 1, NMAX)      0031
   31   FORMAT (1X, A4, 3F8·4)                                             0032
C       FRACTIONAL TO CARTECIAN COORDINATES                                0033
        GO TO (40, 41, 42), NRDCN                                          0034
   40   READ (5, 4) A, B, C, ALFA, BETA, GAMMA                            0035
        CALL RDCONS (NRDCN)                                                0036
        GO TO 41                                                           0037
   42   CALL RDCONS (NRDCN)                                                0038
   41   CONTINUE                                                           0039
        DO 998 NN = 1, NVIEW                                               0040
        READ (5, 2) NZERO, NAXIS, NATOM, (NROT (I), I = 1, 3)              0041
        WRITE (6, 2) NZERO, NAXIS, NATOM, (NROT (I), I = 1, 3)             0042
        READ (5, 4) (PHI (I), I = 1, 3)                                    0043
        WRITE (6, 4) (PHI (I), I = 1, 3)                                   0044
C       ONE OF THE ATOMS IS KEPT AT THE ORIGIN                             0047
        IF (NZERO) 43, 43, 44                                              0045
   44   CONTINUE                                                           0046
        DO 424 J = 1, 3                                                    0048
        ATOM (J) = X (J, NZERO)                                            0049
        DO 424 I = 1, NMAX                                                 0050
  424   X (J, I) = X (J, I)—ATOM (J)                                       0051
C       ONE VECTOR IS PUT ALONG THE DESIRED AXIS                           0052
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43    IF (NAXIS) 45, 45, 46                                          0053
46    DO 451 I = 1,3                                                 0054
451   P (I) = X (I, NATOM)                                           0055
      DENOM= P (1)*P (1) + P (2) *P (2) + P (3) * P (3)              0056
      DENOM = SQRT (DENOM)                                           0057
      GO TO (452, 453, 454), NAXIS                                   0058
452   IJ = 2                                                         0059
      IK = 3                                                         0060
      GO TO 455                                                      0061
453   IJ = 3                                                         0062
      IK = 1                                                         0063
      GO TO 455                                                      0064
454   IJ = 1                                                         0065
      IK = 2                                                         0066
455   CONTINUE                                                       0067
      DENO = SQRT (P (IJ) *P (IJ) + P (IK)*P (IK))                   0068
      TANW = DENO/P (NAXIS)                                          0069
      TETA = ATAN (TANW)                                             0070
      TETA = TETA/CONFA                                              0071
      DC (NAXIS) = 0.0                                               0072
      DC (IJ) = P (IK)/DENOM                                         0073
      DC (IK) = - P (IJ)/DENOM                                       0074
      CALL ROMAX (DC, TETA, AMAT)                                    0075
      DO 466 I = 1, NMAX                                             0076
      DO 47 J = 1, 3                                                 0077
47    X1 (J, 1) = X (J, I)                                           0078
      CALL RMM (AMAT, 3, 3, X1, 1, X1)                               0079
      DO 48 J = 1, 3                                                 0080
48    X (J, I) = X1 (J, 1)                                           0081
466   CONTINUE                                                       0082
45    CONTINUE                                                       0083
      ROTATION OF THE MOLECULE ABOUT ANY AXIS SUCCESSIVELY           0084
      DO 101 I = 1, 3                                                0085
      DO 100 II = 1, 3                                               0086
100   DC (II) = 0.0                                                  0087
      IJK = IABS (NROT (I))                                          0088
      IF (NROT (I) 102, 101, 103                                     0089
102   DC (IJK) = - 1.0                                               0090
      GO TO 104                                                      0091
103   DC (IJK) = 1.0                                                 0092
104   CONTINUE                                                       0093
      ANG = PHI (I)                                                  0094
      CALL ROMAX (DC, ANG, AMAT)                                     0095
      DO 105 J = 1, NMAX                                             0096
      DO 106 K = 1, 3                                                0097
106   X1 (K, 1) X = (K, J)                                           0098
      CALL RMM (AMAT, 3, 3, X1, 1, X1)                               0099
      DO 107 K = 1, 3                                                0100
107   X (K, J) = X1 (K, 1)                                           0101
105   CONTINUE                                                       0102
101   CONTINUE                                                       0103
1052  FORMAT (3 (2X, A4, 3F10.4)/)                                   0104
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      GO TO (1050, 1060), NTYPE                                          0105
 1050 CONTINUE                                                           0106
      WRITE (6, 1053)                                                    0107
 1053 FORMAT (10X, ' COORDINATES FOR ORTHOGRAPHIC PROJECTION '/)         0108
      WRITE (6, 1052) (ANAME (J), (X (I, J), I = 1, 3), J = 1, NMAX)     0109
      GO TO 998                                                          0110
 1060 CONTINUE                                                           0111
      WRITE (6, 1054)                                                    0112
 1054 FORMAT (10X, ' COORDINATES FOR PERSPECTIVE PROJECTION '/)          0113
C     MOLECULE IS SHIFTED TO—Z BY ZMAX. . .                              0114
      JJ = 1                                                             0115
 1012 ZCOR = X (3, JJ)                                                   0116
      IF (ZCOR) 1010, 1011, 1011                                         0117
 1010 JJ = JJ + 1                                                        0118
      GO TO 1012                                                         0119
 1011 CONTINUE                                                           0120
      J2 = JJ + 1                                                        0121
      DO 1013 JJ = J2, NMAX                                              0122
      ZCORI = X (3, JJ)                                                  0123
      IF (ZCORI) 1013, 1014, 1014                                        0124
 1014 CONTINUE                                                           0125
      IF (ZCOR—ZCORI) 1015, 1013, 1013                                   0126
 1015 ZCOR = ZCORI                                                       0127
 1013 CONTINUE                                                           0128
      DO 2010 JJ = 1, NMAX                                               0129
 2010 X (3, JJ) = X (3, JJ)—ZCOR                                         0130
C     CALCULATE THE PERSPECTIVE COORDINATES                              0131
 1044 CONTINUE                                                           0132
      DO 1030 JJ = 1, NMAX                                               0133
      ZA = ABS (X (3, JJ))                                               0134
      DENO = ZSP + ZA                                                    0135
      XR (1, JJ) = (EYE*ZA + X (1, JJ)* ZSP)/DENO                        0136
      XR (2, JJ) = X(2, JJ) * ZSP/DENO                                   0137
 1030 XR (3, JJ) = X (3, JJ)                                             0138
      IF (EYE) 1040, 1041, 1042                                          0139
 1042 EYE = — EYE                                                        0140
      WRITE (6, 332)                                                     0141
      WRITE (6, 1066)                                                    0142
 1066 FORMAT (10X, ' COORDINATES AS VIEWED BY THE RIGHT EYE '/)          0143
      WRITE (6, 332)                                                     0144
      WRITE (6, 1052) (ANAME (J), (XR (I, J), I = 1, 3), J = 1, NMAX)    0145
      GO TO 1044                                                         0146
 1040 WRITE (6, 332)                                                     0147
      WRITE (6, 1067)                                                    0148
 1067 FORMAT (10X, ' COORDINATES AS VIEWED BY THE LEFT EYE '/)           0149
      WRITE (6, 332)                                                     0150
      WRITE (6, 1052) (ANAME (J), (XR (I, J), I = 1, 3), J = 1, NMAX)    0151
      GO TO 998                                                          0152
 1041 WRITE (6, 332)                                                     0153
      WRITE (6, 1068)                                                    0154
 1068 FORMAT (10X, ' COORDINATES FOR SINGLE PERSPECTIVE DIAGRAM '/)      0155
      WRITE (6, 332)                                                     0156
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      WRITE (6, 1052) (ANAME (J), (XR (I, J), I = 1, 3), J = 1, NMAX)        0157
998   CONTINUE                                                               0158
999   CONTINUE                                                               0159
      STOP                                                                   0160
      END                                                                    0161
      SUBROUTINE RDCONS (NRDCN)                                              0162
      DIMENSION ATOM (3)                                                     0163
      COMMON A, B, C, ALFA, BETA, GAMMA, NMAX, X (3, 100)                    0164
      CONFA = 0·01745329                                                     0165
      GO TO (13, 11, 16), NRDCN                                              0166
13    CONTINUE                                                               0167
      PALFA = ALFA*CONFA                                                     0168
      PBETA = BETA*CONFA                                                     0169
      PGAMMA = GAMMA*CONFA                                                   0170
      CA = COS (PALFA)                                                       0171
      CB = COS (PBETA)                                                       0172
      CG = COS (PGAMMA)                                                      0173
      SG = SIN (PGAMMA)                                                      0174
      CPSI = (CB—(CA*CG))/SG                                                 0175
      CRO = SQRT (1·0—(CA*CA + CPSI*CPSI))                                   0176
      DO 14 I = 1, NMAX                                                      0177
      ATOM (1) = X (1, I)* SG*A + X (3, I)* CPSI*C                           0178
      ATOM (2) = X (1, I)* CG*A + X (2, I)* B + X (3, I)* CA*C               0179
      ATOM (3) = X (3, I)* CRO*C                                             0180
      DO 14 J = 1, 3                                                         0181
14    X (J, I) = ATOM (J)                                                    0182
      GO TO 11                                                               0183
16    CONTINUE                                                               0184
      DO 17 I = 1, NMAX                                                      0185
      OMEGA = X (2, I)                                                       0186
      OMEGA = OMEGA*CONFA                                                    0187
      ATOM (1) = X (1, I)*COS (OMEGA)                                        0188
      ATOM (2) = X (1, I)*SIN (OMEGA)                                        0189
      DO 17 J = 1, 2                                                         0190
17    X (J, I) = ATOM (J)                                                    0191
11    CONTINUE                                                               0192
      RETURN                                                                 0193
      END                                                                    0194
      SUBROUTINE ROMAX (DC, ANG, AMAT)                                       0195
      DIMENSION DC (3), AMAT (3, 3)                                          0196
      CONFA = 0·01745329                                                     0197
      ANG = ANG*CONFA                                                        0198
      C = COS (ANG)                                                          0199
      S = SIN (ANG)                                                          0200
      CC = (1·—C)                                                            0201
      AMAT (1, 1) = C + DC (1)*DC (1)*CC                                     0202
      AMAT (1, 2) = DC (1)*DC (2)*CC—DC (3)*S                                0203
      AMAT (1, 3) = DC (1)*DC (3)*CC + DC (2)*S                              0204
      AMAT (2, 1) = DC (1)*DC (2)*CC + DC (3)*S                              0205
      AMAT (2, 2) = C + DC (2)*DC (2)*CC                                     0206
      AMAT (2, 3) = DC (2)*DC (3)*CC—DC (1)*S                                0207
      AMAT (3, 1) = DC (1)*DC (3)*CC—DC (2)*S                                0208
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      AMAT (3, 2) = DC (2)*DC (3)*CC + DC (1)*S                          0209
      AMAT (3, 3) = C + DC (3)*DC (3)*CC                                 0210
      RETURN                                                             0211
      END                                                                0212
      SUBROTINE RMM (A, K, L, B, N, C)                                   0213
      DIMENSION A (3, 3), B (3, 1), C (3, 1), X1 (3)                     0214
      DO 10 I = 1, N                                                     0215
      DO 20 J = 1, K                                                     0216
      X1 (J) = 0·0                                                       0217
      DO 20 KK = 1, L                                                    0218
   20 X1 (J) = X1 (J) + A (J, KK) *B (KK, I)                             0219
      DO 10 J = 1, K                                                     0220
   10 C (J, I) = X1 (J)                                                  0221
      RETURN                                                             0222
      END                                                                0223
```