APPENDIX I

CONVERSION OF COORDINATES FROM ONE SYSTEM TO ANOTHER

USING THE STEREOGRAPHIC PROJECTION METHOD

The method described here makes use of the cyclographic projection technique, which is a slight modification of the conventional stereographic projection method. In the usual stereographic projection, any crystal face can be represented as a point on the stereogram and the angles between the faces can be directly measured on the stereogram using a Wulff net. In the cyclographic projection method, it is the normal to the face that is represented as a point on the stereogram. In other words, any line in space can be represented as a point on the stereogram and all the angular relationships can be directly obtained with a Wulff net.

This method can be used in general, to convert the coordinates of a point in any system to any other system of coordinates. In this appendix, for example, the conversion of coordinates of the atoms in the case of sugars, from the reported system of coordinates to an orthogonal system with C$_3$ as origin, C$_3$O$_5$ as X-axis and C$_3$O$_5$O$_1$ as XY-plane is illustrated. This has been made use of in the evaluation of standard parameters for the sugar residue described in section 2 of Chapter 4.
The first step in the conversion is to project the atoms in a plane perpendicular to an axis. The distances of the various atoms from $C_3$ (which is the origin in the converted system of coordinates) in the projection are noted as $\Delta l$. The difference in the vertical heights of the atoms and that of $C_3$ are also noted as $\Delta h$. Using the Wulff net, the representative points on the stereogram for the various lines joining $C_3$ to the respective atoms are plotted as follows. The representative point corresponding to any atom is plotted at an angle $\phi$ from the circumference of the primitive circle along the line joining the projections of $C_3$ and the atom, with $C_3$ as the centre of stereogram, $\phi$ being given by $\tan^{-1} (\Delta h / \Delta l)$.

In Figure A.1, the representative points corresponding to $C_3C_1$, $C_3C_2$, and $C_3C_4$ are shown. Atoms lying below the plane of projection with respect to $C_3$ (i.e., $\Delta h < 0$) are represented by full circles, while open circles represent the atoms lying above the plane of projection (i.e., $\Delta h > 0$).

It can be seen from Figure A.2, that the coordinates $x$, $y$ and $z$ of any point $R$ is

$$x = l \cos \psi$$

$$y = l \sin \psi$$

and

$$z = l \sin \theta$$

where $l$ is the distance of the point $R$ from the origin, $\Delta x = l \cos \psi$, the projected distance of OR in the $XY$-plane.
FIG. A1

Stereogram showing the representative points of the
planes C_3C_1, C_3C_5, C_3C_4, which form the X Y plane and the
representative point of any other line C_3C_4. The great
circle used for measurement of the latitude $\theta$ and
longitude $\psi$ are also indicated.
FIG. A.2

Diagram showing the relation between the rectangular coordinates $x, y, z$ and the parameters $L, l, \theta$ and $\Psi$. 

• Diagram showing the relation between the rectangular coordinates $x, y, z$ and the parameters $L, l, \theta$ and $\Psi$. 

and \( \varphi \) the angle which the projection makes with the \( x \)-axis. Hence, it is only necessary to find out the two angles \( \psi \) and \( \theta \).

For this, the great circle \( AB \) passing through the representative points \( C_3C_5 \) and \( C_3C_1 \) is first drawn and the stereographic pole \( P \) of this great circle and its inverse \( P' \) are also marked. In fact \( P \) is now the representative point of the line that is normal to the plane \( C_3C_1C_5 \) i.e. the \( z \)-axis. The great circle \( EF \) passing through \( P \) and the representative point of the line joining \( C_3 \) to any other atom (\( C_3C_4 \) in this case) is then drawn to meet the great circle \( AB \) at \( C_3B \). The latitude \( \theta \), which is the angle \( C_3B \wedge C_3C_4 \) measured along the great circle \( EF \) and the longitude \( \psi \) which is the angle \( C_3C_5 \wedge C_3B \) measured along the great circle \( AB \) are then readily obtained for the various atoms, with the help of a Wulff net.
Three programmes were written for the various calculations used in Chapters 1 and 2. These are:
(1) calculation of helical parameters; (2) calculation of distances between the atoms in the two linked peptide residues for evaluating the allowed conformations of the peptides; and (3) evaluation of the parameters (\( \psi, \psi' \)) of the peptide residues in actual di-, tri- and polypeptide structures. While the former two programmes were written in the Autocode language for the digital computer Elliott-803, the third one was written in the Fortran language for the IBM 1620 digital computer.

**Programmes for the Elliott-803 Digital Computer**

Elliott-803 is a digital computer with a memory of 4096 words. Each location can store either one number or two instructions. The input is in the form of paper tape with five holes. The programme written in the auto code is first translated by the computer into the machine code and then executed.

1) **Programme for the Calculation of Helical Parameters**

The programme for the calculation of helical parameters was written in exactly the same way as was done
using the desk calculator. The flow chart incorporating the broad features of the various steps are shown in Figure A.3

2) PROGRAMME FOR CALCULATING NH: CONTACT DISTANCES

This programme also was written for the Elliott-803 digital computer in the autocode language. In fact, this programme consists of two parts. In the first part, the coordinates of the various atoms after rotation through θ and θ' are obtained and the contact distances of the relevant backbone atoms from Cβ, N1 and C2' are also evaluated. The ranges of θ and θ' allowed by the minimum contact distances were then selected manually. In the second part, the input data are the coordinates of the atoms after being rotated through θ and θ' (output of the first part) and the allowed ranges of θ and θ'. The final selection of the allowed combinations of (θ,θ') was also done manually. Figure A.4 give the flow charts for the two parts of this programme.

3) PROGRAMME FOR THE EVALUATION OF (θ,θ') OF AMINO ACIDS AND SIMPLE PEPTIDES

This programme was written in the Fortran language for the digital computer I M 1620. This computer contains 40,000 memory locations, with each memory location containing 6 bits. The information is stored in the binary
A.3. FLOW CHART FOR THE EVALUATION OF HELICAL PARAMETERS.
READ INITIAL CO-ORDINATES OF ATOMS AND CONSTANTS FOR THE TRANSFORMATION RELATIONS

GENERATE COS θ AND SIN θ FOR θ = 90° AT 5° INTERVALS AND STORE

CALCULATE THE COORDINATES OF ATOMS AFTER ROTATION THROUGH φ AND φ' AND PUNCH

SET φ = 0

CALCULATE DISTANCES OF ATOMS C\(_1\), C\(_3\), O\(_1\) AND H\(_1\) FROM C\(_B\) AND C\(_2\) AND PRINT

HAS θ REACHED 180°?

NO

INCREASE φ BY 10°

YES

CALCULATE DISTANCES OF ATOMS O\(_2\), N\(_2\), H\(_2\) AND C\(_3\) FROM C\(_B\) AND N\(_1\) AND PRINT

SET φ = 0

HAS φ' REACHED 180°?

NO

INCREASE φ' BY 10°

YES

STOP

READ TRANSFORMED CO-ORDINATES AND SELECTED RANGES OF φ AND φ'

CALCULATE OTHER CONTACT DISTANCES IN THE ALLOWED RANGES OF φ, φ'

PRINT φ, φ' AND CONTACT DISTANCES

STOP

Figure: Flow chart for the evaluation of distances between atoms in adjacent peptide residues for various values of (φ, φ')

PART II
encoded system and only one digit can be stored in one location. The input for this computer is in the form of punched cards; the programme written in Fortran language is converted into machine code by means of the processor and used for the calculations.

This programme has been used for the evaluation of \( (\phi, \phi') \) for the structures of amino acids, N-terminal, middle and C-terminal residues in di-, tri-peptides and also in the case of polypeptide structures. Figure A.5 represents the flow chart giving the salient features of the programme. The details in individual cases corresponding to the amino acid, N-terminal and C-terminal residues are given below:

a) Amino acids

The only relevant parameters \( \phi_1 \) and \( \phi_2' \) in this case are directly obtained as the angle between the planes \( N_0-C_1-C_1' \) and \( C_1-C_1'-\omega_1 \) (\( \phi_1' \)) and between the planes \( N_0-C_1-C_1' \) and \( C_1-C_1'-\omega_2 \) (\( \phi_2' \)). In order to determine the sign of \( \phi' \) (\( \phi_1' \) or \( \phi_2' \)), the following check is made.

\[
\begin{align*}
N_0 & \rightarrow C_1 \rightarrow C_1' \rightarrow 0 \\
\end{align*}
\]

The three vectors \( \vec{C}_1N_0 \), \( \vec{C}_1C_1' \) and \( \vec{C}_10 \) are designated as \( \vec{x}_1 \), \( \vec{x}_2 \) and \( \vec{x}_3 \) and the normals to the plane...
Figure 25: Chart showing the salient features of the programme written for evaluation of $(\phi, \phi')$ in actual structures.
$N_0 - C_1 - C_1'$ and $C_1 - C_1' - 0$ by $\vec{R}_1$ and $\vec{R}_2$ respectively such that

$$\vec{R}_1 = \vec{r}_1 \times \vec{r}_2$$

and $$\vec{R}_2 = \vec{r}_2 \times \vec{r}_3$$

The direction of the vector $\vec{R}_1 \times \vec{r}_2$ is compared with that of $\vec{r}_2$. If both are the same, then $\phi'$ lies between $0^\circ$ and $180^\circ$ and if the two directions are opposite, then $\phi'$ lies between $0^\circ$ and $-180^\circ$. The flow chart for this case is shown in Figure A.6.

b) X-terminal residues

![Diagram](image)

The parameter $\phi'$ is the angle between the plane $N_0 - C_1 - C_1'$ and the plane which passes through $C_1$ and $C_1'$ and fitting best with the other atoms, namely, $O_1$, $N_1$, $H_1$ and $C_2$. This best plane is obtained by minimizing the sum of the squares of the deviations of these atoms. The relevant direction of the normal to this plane is found out by comparing it with the direction of the vector $(\vec{c}_1 \vec{c}_1' \times \vec{c}_1 \vec{c}_1')$. The sign of $\phi'$ is determined in the same way as in the case of amino acids. The flow chart in this case is shown in Figure A.7.
FIG. A-6 FLOW CHART FOR EVALUATING $\phi'_1$, $\phi'_2$ FOR AMINO ACIDS.
Fig. A.7. Flow chart for evaluating \( \phi' \) N-terminal residues.
e) C-terminal residues

The parameter $\phi$ in this case is the angle between the planes $N_0-C_1-C_1'$ and the plane passing through $C_1N_0$ and fitting best with $N_0$, $C_1'$, $O_0$, and $C_0$. The relevant direction of the normal to this plane is found by comparing it with the direction of the vector $(\vec{C}_1C_0' \times \vec{C}_1N_0)$. The sign of $\phi$ is determined by comparing the vector $(\vec{R}_1 \times \vec{R}_2)$ ($\vec{R}_1$, $\vec{R}_2$ being the vectors representing the normals to the planes $N_0-C_1-C_1'$ and the plane obtained by best fit) with $C_1N_0$. The parameters $\phi_1$, $\phi_2$ in this case are calculated in exactly the same way as in amino acids. The flow chart for this case is shown in Figure A.8.

d) Middle residues

In this case the parameter $\phi$ is calculated in exactly the same way as for the C-terminal residue and the parameter $\phi'$ in the same way as for the N-terminal residue.
G.A.O. FLOW CHART FOR EVALUATING $\phi$, $\phi_1'$, AND $\phi_2'$ FOR C-TERMINAL RESIDUES