**Laboratory Notes**


**Measurement of the atomic coordinates of a Kendrew-type model from two projections**

A very simple method for measuring coordinates of a Kendrew model is described. It consists of measuring the planar coordinates of two projections of the model. The accuracy is excellent: the e.s.d. of the backbone bond lengths is less than 0.07 Å.

**Principle of the method**

The principle of the method, basically analogous to the photographic one described by Iga, Kusunoki, Yasuoka & Kakudo (1982), consists of measuring the planar coordinates of two different model projections. One uses a point light source in order to get an acute shadow on a screen (Fig. 1). The coordinates X, Y, Z and x, y, respectively, of a point M and of its shadow m on the screen are related by

\[
x' = X / (Z + 1); \quad y' = Y / (Z + 1),
\]

where the following reduced coordinates have been defined:

\[
x' = x / d, \quad y' = y / d, \quad X' = X / d, \quad Y' = Y / d, \quad Z' = Z / d.
\]

(D, d given in Fig. 1 as SO’, SO) Rotating the model by θ around the OX axis, a point M(xo, yo, zo) becomes M’(x’o, y’o, z’o). Straightforward geometrical considerations lead to the linear system of equations with X, Y, Z as unknowns:*  

\[
X' - x'Z = x' \\
y' - y'Z = y' \\
x'' - x''Y \sin \theta - x''Z \cos \theta = x'' \\
(\cos \theta - y'' \sin \theta) Y' = y' - (y'' \cos \theta + \sin \theta)Z' = y''.
\]

**Practical setup**

We have used as light source a simple slide projector with a front pupil (O

\[\text{Fig. 1. Geometry of the system. S: point light source; SO': normal line to the screen onto which the model is projected; OXYZ: coordinate system in which calculations are done; O'xy: screen coordinate system; OX: rotation axis of the model; distances SO = d, SO' = D.}\]

---

**Table 1. Minimum, maximum and mean values (with e.s.d.) for bond lengths (Å) and torsion angle around the peptide bond (°)**

<table>
<thead>
<tr>
<th>Bond</th>
<th>Minimum value</th>
<th>Mean value</th>
<th>Maximum value</th>
<th>Standard value</th>
</tr>
</thead>
<tbody>
<tr>
<td>N—CA</td>
<td>1.14</td>
<td>1.49(0.07)</td>
<td>1.61</td>
<td>1.45</td>
</tr>
<tr>
<td>CA—C</td>
<td>1.68</td>
<td>1.56(0.06)</td>
<td>1.84</td>
<td>1.51</td>
</tr>
<tr>
<td>C—O</td>
<td>1.06</td>
<td>1.20(0.06)</td>
<td>1.40</td>
<td>1.24</td>
</tr>
<tr>
<td>C—N</td>
<td>1.06</td>
<td>1.32(0.06)</td>
<td>1.54</td>
<td>1.32</td>
</tr>
<tr>
<td>Torsion angle</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CA—C—N—CA</td>
<td>160°-7</td>
<td>180°1(8-2)</td>
<td>203°6</td>
<td>180°0</td>
</tr>
</tbody>
</table>

*Obviously only three of these four equations are independent. This can be expressed by equating to zero the determinant of coefficients which yields*

\[
tan(\theta/2) = (x' - x''_o) / (y' + y''_o).
\]

This equation is of little practical interest owing to very bad precision because both the numerator and the denominator are often close to zero.

---

**Results and discussion**

We have used this method to measure the coordinates of a small protein, a cardiotoxin from Naja Mossambica Mossambica (Mr = 6700). The analysis of results reported in Table 1 has been done on the skeleton atoms N, CA, C, O, so it is probably slightly over-optimistic for the whole molecule, owing to possible small displacements of side chains. It is nevertheless quite representative of the intrinsic quality of the method. We noticed also the fact already underlined by Frentrup & Tulinsky (1981) that mean bond lengths N—CA and CA—C are larger than the standard values because of the mechanical junction in the Kendrew models. On the other hand, the mean C—N bond length, 1.321 Å, is very near the standard value, 1.325 Å.

Overlapping of many bonds producing some ill-defined shadows can be a real drawback for both accuracy and rapidity. To overcome this difficulty for larger molecules, where such superpositions become more frequent, it is always possible to use the general method described above, choosing different orientation angles for different groups of atoms. A simpler way of solving the
 problem is to point at an atom of the model from two different directions and to extrapolate the shadows of the pointer on the screen.

PHILIPPE DUMAS
BERNARD REES

Laboratoire de Cristallographie
Biologique
Institut de Biologie Moleculaire et
Cellulaire du CNRS
15 rue Rene Descartes
67084 Strasbourg CEDEX
France

References

Crystallographers

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography, J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Professor D. A. Bekoe, Legon, Accra, Ghana, has become Director of the Unesco Regional Office for Science and Technology for Africa. Sir John Kendrew, St John's College, Oxford, England, has succeeded Professor Bekoe as President of the International Council of Scientific Unions.

Dr Norman F. M. Henry died on 10 July 1983 at the age of 73 after some years of failing health. He graduated at the University of Aberdeen but spent the rest of his working life in the Department of Mineralogy and Petrology (now the Department of Earth Sciences) in the University of Cambridge. Dr R. C. Evans writes that there he made major contributions to the teaching of physical and chemical crystallography and in his time was responsible with his colleagues for introducing the subject to several thousand students, possibly more than any other single laboratory in the world. Some of his teaching material he published in 1951 (jointly with H. Lipson and W. A. Wooster) in The Interpretation of X-ray Diffraction Photographs, a second edition of which appeared in 1960.

Henry's research interests were in the field of reflected-light optics, and in collaboration with R. Galgon he published Microscopic Study of Opaque Minerals in 1972. He also edited and prepared for press the third edition of A. F. Hallmond's The Polarizing Microscope. Crystallographers worldwide will, however, best remember Henry for his work for the Union and particularly for International Tables for X-ray Crystallography. He was a member of the Commission for these Tables from its inception in 1948 until 1972 and Chairman for eight of these years. As Editor (jointly with Dame Kathleen Lonsdale) of the first volume to appear he played a large part in deciding the content of the several volumes and, no less important, in cooperating with the printers in an extensive series of experiments to develop a format not only elegant but also appropriate to the diverse and specialized material involved. Only those who saw him at work day to day can be aware of the years of meticulous effort that he devoted to this task. When Chairman of the Commission Henry was an ex-officio member of the Commission on Crystallographic Nomenclature; he was also Chairman for three years of the Commission on Crystallographic Teaching.

Henry was a man of taste and discernment with a lively interest in literature, music, the arts and gastronomy. His knowledge of wine served him well in his office as Steward of St John's College, of which he was a Fellow, and during his tenure of that office it was characteristic of him that he should have founded a Food and Wine Society to encourage undergraduate students to share the delights that gave him so much pleasure. His years of retirement, from 1977, he spent in College and during these years he applied his editorial expertise to the preparation of a College Register. It was he, too, who was largely responsible for encouraging one of his colleagues to write an architectural history of St John's College, a work to the preparation of which Henry made notable contributions.

Dr Rose C. L. Mooney Slater died 21 November 1981 at her home in Gainesville, Florida. Born in New Orleans in 1902, she received her BS in 1926 and MS in 1929 from Tulane University and her PhD in physics from the University of Chicago in 1932. Dr Elizabeth A. Wood writes that, after teaching physics at Newcomb College of Tulane University from 1926 to 1952, Rose Mooney Slater worked at the National Bureau of Standards from 1952 to 1956 and then as a research physicist and associate at M.I.T. from 1956 to 1968. When she retired in 1974 she had been a research professor of chemistry at the University of Florida for eight years. She is remembered by her colleagues and students as a warm-hearted and gracious person who combined the charm of her New Orleans background with the competent integrity of a scientist. She was the author of many articles on the determination of the structure of crystals and crystalline materials by X-ray diffraction, and was a charter member of the American Crystallographic Association and a Fellow of the American Physical Society.

Dr Chung Soo Yoo, a member of the Biocrystallography Laboratory of the Veterans Administration Medical Center in Pittsburgh and Research Associate in the Department of Crystallography at the University of Pittsburgh, was killed when Korean Airline Flight 007 was shot down on 31 August 1983. Dr Martin Sax writes that Dr Yoo came to the USA in 1965, obtained his MS degree in chemistry at Rice University in 1967, his PhD in crystallography at the University of Pittsburgh in 1971, and became a US citizen. He was working on the structures of macromolecules and at the time of his death was traveling to Korea to give a series of lectures on X-ray crystallography at Kang Wan National University. Dr Yoo was a popular and highly respected scientist who will be sorely missed by his many friends and colleagues.

International Union of Crystallography

Prices of Acta Crystallographica and Journal of Applied Crystallography

The Executive Committee of the International Union of Crystallography is pleased that it has only been necessary to make a slight increase to the regular price subscription rates and the prices of back numbers for Acta Crystallographica and Journal of Applied Crystallography as from 1 January 1984. The subscription rates for personal copies are unchanged.

Acta Crystallographica

The following rates will apply for volumes A40, B40 and C40 (1984). Note that, except as single parts, Sections B and C are only available together. All subscription rates are fixed in Danish kroner, and the US dollar equivalents given below are subject to exchange-rate fluctuations and amendment without notice.