The Braggs and the Foundations of Modern Crystallography

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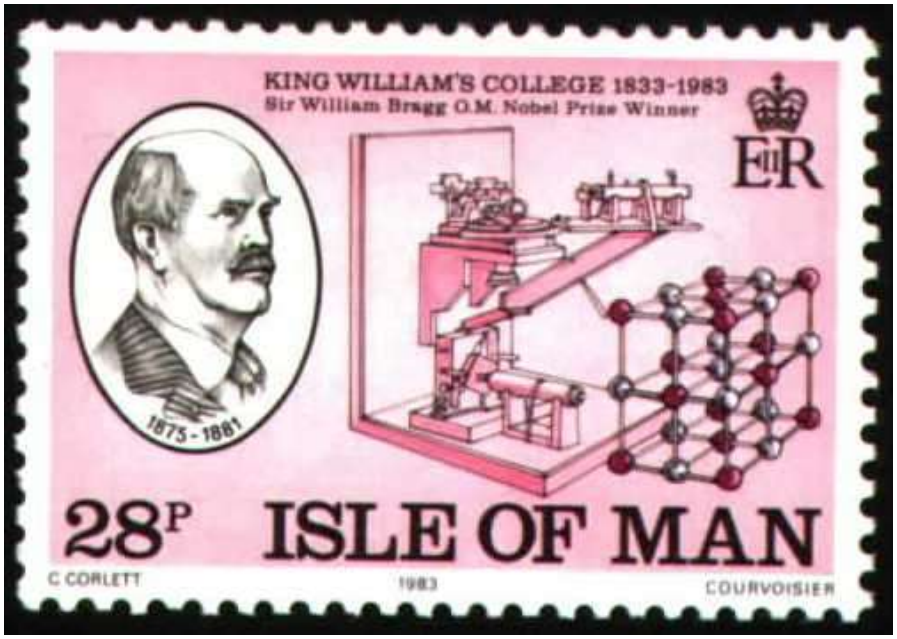

KING WILLIAM'S COLLEGE 1833-1983
Sir William Bragg O.M. Nobel Prize Winner
E II R
1875 - 1881
28P ISLE OF MAN
C CORLETT
1983
COURVOISIER


60c AUSTRALIA
2012
William Lawrence Bragg
The Nobel Prize
in Physics 1915
Sir William Dargie

W. L. Bragg

The Structure of Beryl, $Be_3Al_2Si_6O_{18}$.

By W. Lawrence Bragg, F.R.S., Langworthy Professor of Physics, Manchester University, and J. West, John Harling Fellow, Manchester University.

(Received May 21, 1926.)

1. The structure of beryl, described in this paper, has some interesting features. In the first place, the ratio of silicon to oxygen atoms in the molecule is that of a metasilicate. As far as we know, no other example of a metasilicate has as yet been completely analysed (Wyckoff* has made some measurements on diopside $MgCa(SiO_3)_2$, but has only succeeded in determining its space group).

The Effect of Thermal Agitation on Atomic Arrangement in Alloys.

By W. L. Bragg, F.R.S., and E. J. Williams, D.Sc., Manchester University.

(Received December 29, 1933.)

Forming the subject of the Bakerian Lecture by Professor W. L. Bragg, F.R.S. (Read June 28, 1934.)

Introduction.

When two metals are alloyed together in various proportions, a series of solid phases is formed. A characteristic phase diagram of a binary alloy system has regions of single phase, throughout which the alloy is homogeneous, alternating with regions in which two neighbouring phases coexist. The com-

The Determination of Parameters in Crystal Structures by means of Fourier Series.

By W. Lawrence Bragg, M.A., F.R.S., Langworthy Professor of Physics, Manchester University.

(Received February 9, 1929.)

1. *Introduction.*

The Fourier representation of the results of X-ray analysis was first suggested by W. H. Bragg.* It was developed independently by Duane, and used by Havighurst and Compton† to give striking representations of the distribution of scattering matter in crystals. Duane and Havighurst were first in applying the method to the much more accurate X-ray measurements available in 1925, and in showing how useful it could be.

The structure of haemoglobin

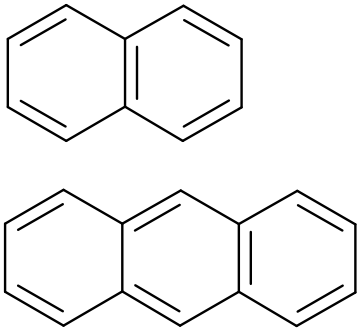
Sir Lawrence Bragg, F.R.S., *Cavendish Laboratory, University of Cambridge* and M. F. Perutz, *Medical Research Council Unit for the Study of the Molecular Structure of Biological Systems, Cavendish Laboratory, University of Cambridge*

(*Received* 20 *February* 1952)

The paper describes the first steps in an attempt to solve the structure of a haemoglobin molecule by X-ray analysis, using a direct method. It is based on an extensive series of absolute measurements of the diffraction by various shrinkage stages of a haemoglobin crystal, and estimates based on many crystalline forms of the general dimensions of the haemoglobin molecule. The methods used are described here and applied to a direct determination of the electron density in one particular direction in the molecule. The extension of the methods to the subsequent problem of obtaining a picture of the molecule as projected on a plane will, it is hoped, form the subject of a subsequent paper.

W. H. Bragg

- E. G. Cox
- K. Lonsdale
- J. D. Bernal
- J. M. Robertson
- R. E. Gibbs
- W. T. Astbury
- C. F. Elam

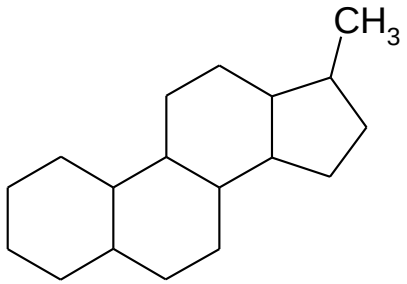


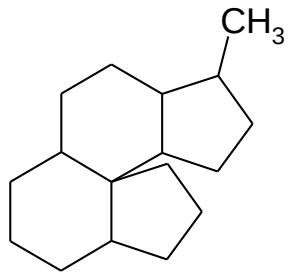
Molecules and Crystals (1921)

Applied to naphthalene and anthracene, the new method was immediately successful in determining that the long axes of the molecules are nearly coincident with the *c* crystal axes. It is obvious that while *a* and *b* remain almost the same in the two unit cells, the *c* axis increases in length by about 2.5 Å in passing from naphthalene to anthracene. Now if the extra ring required by the chemical formula has the dimensions of the rings of carbon atoms found in diamond or graphite, it would account for this addition of about 2.5 Å.

Although this study of hydrocarbons is by no means complete, the essential similarities of the crystal structures and the comparative methods of arriving at molecular dimensions already justify the value of such *extensive crystallographic surveys. The more substances* studied in this way, the more diverse and certain will be the deductions drawn from the crystallographic data.

J. Chem. Soc. 93, 1935





21. *The Structure of Some Hydrocarbons related to the Sterols.*

By J. D. Bernal and (Miss) D. Crowfoot.

The structural formulæ of the sterols and related bile acids and œstrogenic hormones have largely been based on their dehydrogenation to polycyclic aromatic hydrocarbons (see *Ann. Reports*, **1933**, **30**, 199). The formulæ are not definitely established in detail, beyond the fact that all contain a phenanthrene nucleus.

THE MEASUREMENT OF BOND LENGTHS IN CONJUGATED MOLECULES OF CARBON CENTRES

BY J. M. ROBERTSON, F.R.S.

I believe there are at least two good reasons for choosing this subject for my contribution. In the now fairly long history of the science of X-ray crystal analysis the aromatic hydrocarbon structures play quite an interesting part. Naphthalene and anthracene, for example, were among the very first organic crystals to be examined by the X-ray method, although they were certainly not the first organic

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Crystal Structures of Polynuclear Aromatic Hydrocarbons. Classification, Rationalization and Prediction from Molecular Structure

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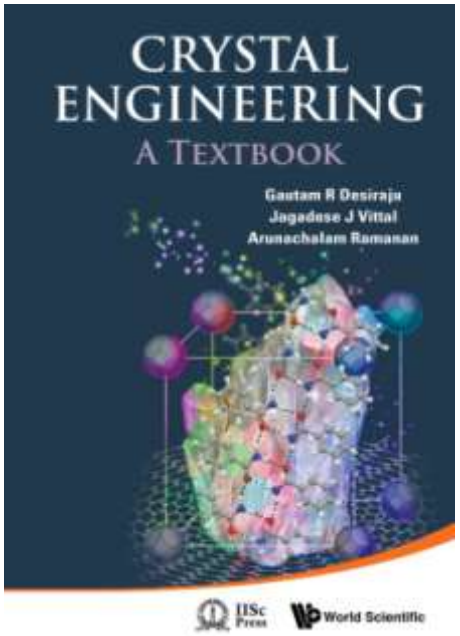
385. *Topochemistry. Part III.*[1,2] *The Crystal Chemistry of some* trans-*Cinnamic Acids.*

By G. M. J. Schmidt.

The crystal structures of substituted cinnamic acids can be divided into three groups (α,β,γ) according to their cell dimensions. These structure groups coincide with the three types of photochemical behaviour reported in Part II: dimerisation to (1) α-truxillic or (2) β-truxinic acid, and (3) light-stability.

X-Ray analyses of members of the α- and β-classes indicate that in these photo-active structures the conformation of the dimers can be correlated with the packing arrangement of nearest-neighbours in the monomer lattice: dimerisation takes place at >C=C< separations of 3·6—4·1 Å and preserves in the (molecular) symmetry of the cyclobutane derivative the (crystallographic) symmetry element relating nearest-neighbour monomers. The separation between >C=C< of 4·7—5·1 Å in the light-stable γ-structures is interpreted as too long for dimerisation to be possible.



Acc. Chem. Res. **1995,** *28,* 193–200

Disappearing Polymorphs

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