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The use of 'Hollerith'* Computing Equipment in Crystal-Structure Analysis†

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The paper gives a brief description of the Hollerith punched-card system of computing from the point of view of the X-ray structure analyst. The principal differences between American and British equipment are described and technical terms in common use are explained.

X-ray structure analysis, with its unrivalled combination of detail and precision, has made a unique contribution to the development of chemistry, but it has been apparent for some time that if it is to continue to play its part in the forefront of chemical progress, the labour of calculation must be reduced by the introduction of systematic computing methods. It seems likely, as interest centres on more and more difficult problems of molecular structure, that for the reasons mentioned below increasing use will be made of punched-card equipment, either in the form of the electromagnetic machines of the present or the electronic machines of the future.‡ Although the Hollerith system may not necessarily be as efficient for a particular calculation as a specially designed machine, it is well-established, reliable and widely distributed throughout the world. Many large industrial and commercial concerns in the U.S.A. and Europe have Hollerith departments, and it is often possible for them to set aside some of their equipment for the use of the scientist for limited periods of time. Probably one of the greatest single advantages of the equipment from the point of view of the X-ray crystallographer is that by means of the interchangeable control panels the machines can be rapidly diverted from one type of calculation to another without delay or inconvenience; it means that any free *machine time* in a statistical department can be made available for scientific use without interference with the normal working of the department.

Hollerith machines have already been used for the computation of Fourier syntheses by several laboratories in the U.S.A. and Britain, and it is natural that crystallographers who have succeeded in obtaining access to machines for this purpose should wish to use them for other calculations. This tendency is in fact shown in the present number of *Acta Crystallographica*, which contains descriptions of two American methods for the calculation of structure factors and of a British method for differential Fourier syntheses. It therefore seems appropriate to give, for the benefit of readers unfamiliar with the Hollerith system, a brief explanation of some of the more standard technical expressions and of the principal differences between British and American machines.

The American (IBM) and the British (BTM) machines use the same *punched-card* principle of expressing the data in the form of holes in cards. In all machines, the punched cards are passed between a metal roller and a series of wire brushes, which make contact to complete electrical circuits only through the punched holes of the cards; exactly which circuit is completed by a hole in a particular position on the cards depends, in the more complicated machines, upon the distribution of plugs in a control panel. The Hollerith operator, by changing the distribution of the plugs in these control panels or *plug-boards* (which resemble miniature telephone switchboards), can make the machine perform any combination of operations within its capacity. This ensures the maximum flexibility in the use of the machines, and, since the plug-boards themselves are detachable, it is possible by wiring spare plug-boards in advance to switch the machines rapidly from one application to another.

The 'Hollerith' card is standard throughout the world. It has eighty vertical columns, in any one of which a number between 0 and 9 can be indicated by a punched hole at the appropriate level. In addition, holes can be punched at two levels above those shown on the printed card, as indicated in Fig. 1, which is a $\frac{3}{4}$-size reproduction of an actual card. This is called *overpunching* in the 'x' and 'y' positions, or simply *x-punching* or *y-punching*. (In Britain, commercial operators often use the x and y positions for tenpence and elevenpence.)

* For convenience we use the name 'Hollerith' in a general sense to describe equipment made both by the International Business Machines Corporation Incorporated (IBM) and by the British Tabulating Machine Co. Ltd. (BTM). Although H. Hollerith did his pioneer work in the U.S.A., usually only equipment made by BTM and its associated companies actually carries his name, American machines being named 'International' or 'IBM'.

† *Editorial note.* This article has been prepared at the request of the Editor to serve as an introduction to a group of papers on the application of punched-card methods in crystal-structure analysis, and is intended for the benefit of readers not familiar with the use of Hollerith and IBM machines. The Editor's thanks are due to the authors for their willingness to write this article.

‡ The latest American calculating punch, Type 604, adds, subtracts, multiplies and divides by electronic means.

For the purpose of planning and describing a computation, the eighty columns of the cards are regarded as being divided in suitable *groups* or *fields*. The holes punched in a *descriptive* or *indicative field* give operational instructions to the machines, while those in an *additive field* represent the numbers on which the arithmetical operations are performed. There is no restriction in the arrangement of the indicative and additive fields, and this is planned for the most economical use of cards and machine time. In complicated methods a particular field on a card may be indicative for one part of the calculation and additive for another. In scientific calculations the x and y over-punching is used only for indicative purposes.

First, the BTM Co. supply a *rolling-total* tabulator which has no American counterpart.* On this machine numbers can be rolled from one counter to another on instruction from an indicative column of the cards. A consequence of this is that the well-known Hollerith method of *progressive digiting* as a means of combined addition and multiplication is likely to be more used by British workers, since it can be done in a single operation on a rolling-total machine (cf. Cox, Gross & Jeffrey, 1949, method (*b*)). It is also possible to roll a counter into itself, and for that reason methods using the numerical data in the binary scale are very effective (Greenhalgh & Jeffrey, unpublished).

The second difference between American and British

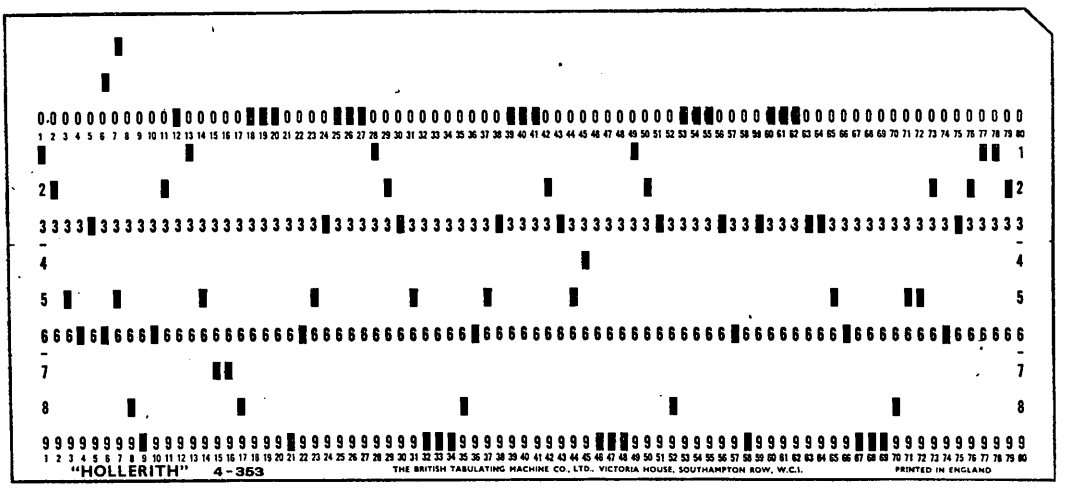

Fig. 1. A typical card, three-quarters original size.

The Hollerith equipment which may be available to the crystallographer consists of the following machines:

(1) *key punch*;
(2) *sorter*;
(3) *reproducing punch* (*comparing reproducer*);
(4) *multiplying punch* (*calculating punch*);
(5) *tabulator* (when fitted with the usual printing mechanism alternatively referred to as an *accounting machine*);
(6) *collator* (this machine performs card selecting and merging operations and although potentially useful for crystallographic calculations, its use is not essential in any of the methods hitherto described).

With the exception of the key punch, which is a machine operated manually, rather like a typewriter, for punching holes in cards, these machines are fully automatic. Several descriptions of the equipment suitable for the general reader have been published (e.g. Eckert, 1940; Comrie, Hey & Hudson, 1937).

With minor modifications, all American and British equipment is the same with the exception of the tabulator, where there are three important differences which must be taken into account in applying IBM methods to BTM tabulators or vice versa.

tabulators is that the former are capable of direct subtraction of negative numbers (which are usually indicated by x-punching above the additive fields). British tabulators subtract by adding 'Hollerith' complements (i.e. complements to 9999...). In practice this means that to represent a quantity to the same number of significant figures in an additive field, one more column is required on cards to be used in BTM tabulators.

The third major difference is that in the American tabulators there is much more flexibility in the allocation of counting wheels into counters. Presumably owing to the requirements of sterling accounting in Britain, the majority of BTM tabulators contain six eleven-wheel counters, the right-hand three wheels of each being specially designed for shillings and pence. It would therefore require a complete change in design to redistribute the counting wheels for the convenience of a particular kind of calculation, and this applies also to the small proportion of British machines which are built for decimal computing.

* This may not now be true, since IBM have recently introduced two new tabulators, Models 402 and 403, which are capable of transferring totals at control changes.

A further consequence of a sterling monetary system is that the multiplying punch, which cannot at present multiply £.*s.d.*, is probably not as popular in Britain as America. A research department in Britain, therefore, which relies on the free time of an industrial statistical department may not have access to the equipment necessary for calculating structure factors by the two methods described in this number.

It is inevitable that a number of technical expressions should appear in the descriptions of the Hollerith methods, and since many of them refer to the same operation whether IBM or BTM equipment is used, it may be useful to extend our explanation to some other common terms.

A tabulator is capable of two distinct operations:

(1) *Listing:* reading information directly from a series of cards and printing it in the form of a table. There is no arithmetical process involved; in fact the counting mechanism is not used.

(2) *Tabulating:* this describes any operation in which data are transferred from the cards to the counters and ultimately printed in tabular form as sub-totals or totals from groups of cards. If the tabulator is coupled to a reproducing punch and the subtotals or totals are punched in a new set of cards, the operation is called *summary-punching*. Tabulating and summary-punching can be done simultaneously.

The cards which are fed into the tabulator for 'listing' or 'tabulating' are called the *detail cards*. In the preparation of the detail cards it may be necessary to use other cards, but there appears to be no standard nomenclature for these. For example, *parameter cards* are referred to in all three papers in this number, and although they all have atomic parameters punched on them, their use in preparation of the detail cards is different in each case. If, however, cards used in the preparation of detail cards are such that they perform the same function in all applications of the method, then they are usually called *master cards*. The *master packs* in the three methods which follow are all the familiar ϕ, $\cos 2\pi\phi$, $\sin 2\pi\phi$ tables in punched-card form. Their function is to punch in a detail card the trigonometric function of the ϕ value which is already present on that card. The process of transferring information from a master card to a series of detail cards is called *gang-punching*, and is done by the reproducing punch. For *intersperse gang-punching*, or *x master-card punching*, the master cards and detail cards are arranged in an appropriate order in a single pack and passed through a suitably controlled reproducing punch, whereupon the required information from each master card is punched into the detail cards which follow it until the arrival of the next master card gives new instructions to the machine. In order that the machine shall distinguish between master cards and detail cards, the former are x-punched in one or preferably two columns.

The term *cross-footing* is an accounting expression taken over to describe the process of adding numbers which are punched in different fields of the same card. It is a special feature of the multiplying punch that it will not only form products of numbers on one card but also add or subtract those products and punch the results on the same card. Such 'cross-footing' operations are impossible on a non-rolling total tabulator and are very inefficient on a rolling-total machine.

Since the details of punched-card equipment are necessarily unfamiliar to many readers, it is desirable that crystallographers publishing accounts of their methods should adopt a standardized terminology as far as possible. We hope that our brief account, which explains many of the terms now used by the Hollerith companies, will not only provide a convenient glossary for the non-technical readers of papers such as those which follow but will also assist in the preparation of papers in this field.

In publishing their computing methods crystallographers have not so far attempted to give instructions for wiring plug-boards and for other machine operations. We do not think it desirable that they should, for in the first place the operation of these machines can only properly be carried out by persons who have been properly trained, and secondly, because, in our experience, if the computational requirements are described in non-crystallographic terms to the Hollerith operator, he can produce the plug-board diagrams best adapted for doing the calculations on his particular types of machines.

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