A Chemical Teletype*

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A Teletype Model 37 machine has been modified for the coding of chemical structures. The coding rate of this machine is higher than that of other machines of this type.

The mechanical coding of chemical structures was introduced in the early 1960's.[1] It was achieved by furnishing a typewriter, first with an appropriate font, and second, with a means for coding both the typed characters and their locations on the typewritten page.

The first machines achieved this positional coding by sensing coordinates. As typewriters equipped with a so-called "reverse line feed" became commercially available, an alternative method, yielding equivalent information, became attractive. In this method, all function keys—i.e., back space, line advance, reverse line feed, etc.—generate codes, and all positioning is done through the use of these keys alone.[2] From the coded sequence, the position of each typed character is therefore readily deduced.

Subsequently, keyboard operated CRT consoles have become available, some of which are amenable to font modification. On these machines, positional information is always obtained, as the displays are controlled by coordinates. A refinement, applicable to this type of machine, allows the computer to assist the operator of the machine in the drawing of the chemical structure.[3]

THE SELECTION OF A MACHINE FOR CHEMICAL INPUT

Since the machines originally developed for the Walter Reed information system[4] were approaching their normal retirement, possible replacements were investigated.[5] The choice between mechanical devices (typewriters) and electronic ones (CRT's) was resolved mainly on the basis of initial cost. The greater speed of the CRT's, when operated as remote terminals, was not taken into account, as the intended use of these machines was predominantly for input, which is an operation limited by typing speed. The error correction problem, a disadvantage of tape typewriters, also was deemed of little account, as it is minimized in positional coding,[6] as well as through the use of magnetic (erasable) tape. The refinement of computer assisted drawing, not being commercially available, was not considered.

Of the typewriters considered, the Teletype Model 37 was selected. Its decisive advantage was its availability with a 126-character complement, which allowed the addition of the required chemical symbols without sacrificing the original characters. In fact, even after all required chemical characters are added, space remains for additional symbols. Use has been made of this extra capacity to introduce symbols to reduce the typing effort. This aspect will be discussed in the next section.

The desirability of the Teletype machine is further enhanced by its line transmission capabilities.

MODIFICATIONS

For ease of subsequent servicing, the basic Teletype machine was modified as little as possible. Since the machine is obtainable with a "reverse line feed" function, it was adapted to the indirect method of coding character positions. Consequently, the machine obtained differs from production models only in the substitution of a "chemical" type box for the standard one.

The machine comes normally with a 6-row type box, holding 96 characters. An 8-row box, containing about 30 spaces for optional characters, is available as an alternative. The modifications undertaken on the Teletype involved the placement of a chemical font into this box. The box can be replaced with another one, by a typist, in a matter of seconds. In this manner, a conventional teletypewriter is always available.

The font for typing chemical structures, which was originally proposed by H. P. Luhn, requires 10 symbols (Figure 1). Deducted from the Teletype's 30 optional spaces, this leaves about 20. Some of these spaces were used for certain Greek characters and other necessary symbols. The remaining spaces were used, as already mentioned, in an arrangement of the chemical symbols to facilitate greater typing efficiency. This is a very important consideration, as the typing of two-dimensional diagrams on an essentially linear typewriter is difficult and time consuming and as the amount of input tends to be large.

Greater typing efficiency was obtained in a number of ways. To minimize the need for case shifting, certain chemical symbols were made available in duplicate and placed in different cases. Reduction in the number of keystrokes was achieved also by carrying two symbols on one type pallet, where experience had shown these symbols to be used frequently in juxtaposition. Finally, some of the optional spaces were sacrificed to extend the pallets of the adjacent row. This arrangement reduces the need for switching back and forth between lines. The details of these arrangements are shown in Figure 2, and the type box implementing them is illustrated in Figures 3 and 4. That these arrangements result in substantial improvement of typing speed, compared with earlier arrangements, is evident from the keystroke counts in Figure 5. (A patent for this chemical font is being applied for. The process for coding chemical structures by means of machines such as

*The findings in this report are not to be construed as an official Department of the Army position.

Figure 1. Basic chemical symbols

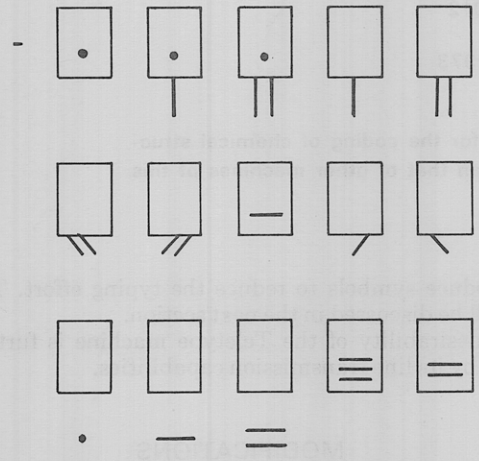

Figure 2. Locations of chemical symbols on type pallet. The frame represents the normal size of the type pallet. To accomodate the symbols outside the frame, the pallets had to be extended

the one described here, is covered by U. S. patents 3,358,804 and 3,476,311. With the exception of the U. S. Government, potential users of such machines and of this process must obtain a license from the author.)

Keyboard layout is governed by human factor considerations. The aim was to achieve a layout where characters typed in succession are typed with alternating hands, and where frequently occurring characters are positioned so that they will be actuated by the first fingers of each hand. The layout is shown in Figure 7, and the corresponding code chart in Figure 8.

COMPARISON WITH THE EARLIER MACHINES

The "chemical" teletypewriters operate under somewhat greater constraints than the custom-made Mergenthaler machines, which they replace. Nevertheless, the output of these different machines is compatible, subject only to algorithmic conversion.

One difference between the above machines results from the need to confine all extended characters to the top row of the type box of the teletypewriter (Figure 3). This arrangement necessarily has its counterpart on the keyboard, so that the Mergenthaler keyboard arrangement could be duplicated only partially.

The teletypewriter also has the odd characteristic that, for a case shift to and from the chemical symbols ("shift in" and "shift out"), as well as for some other functions, it requires the actuation of two keys. The Teletype Company did develop a single keystroke control for these func-

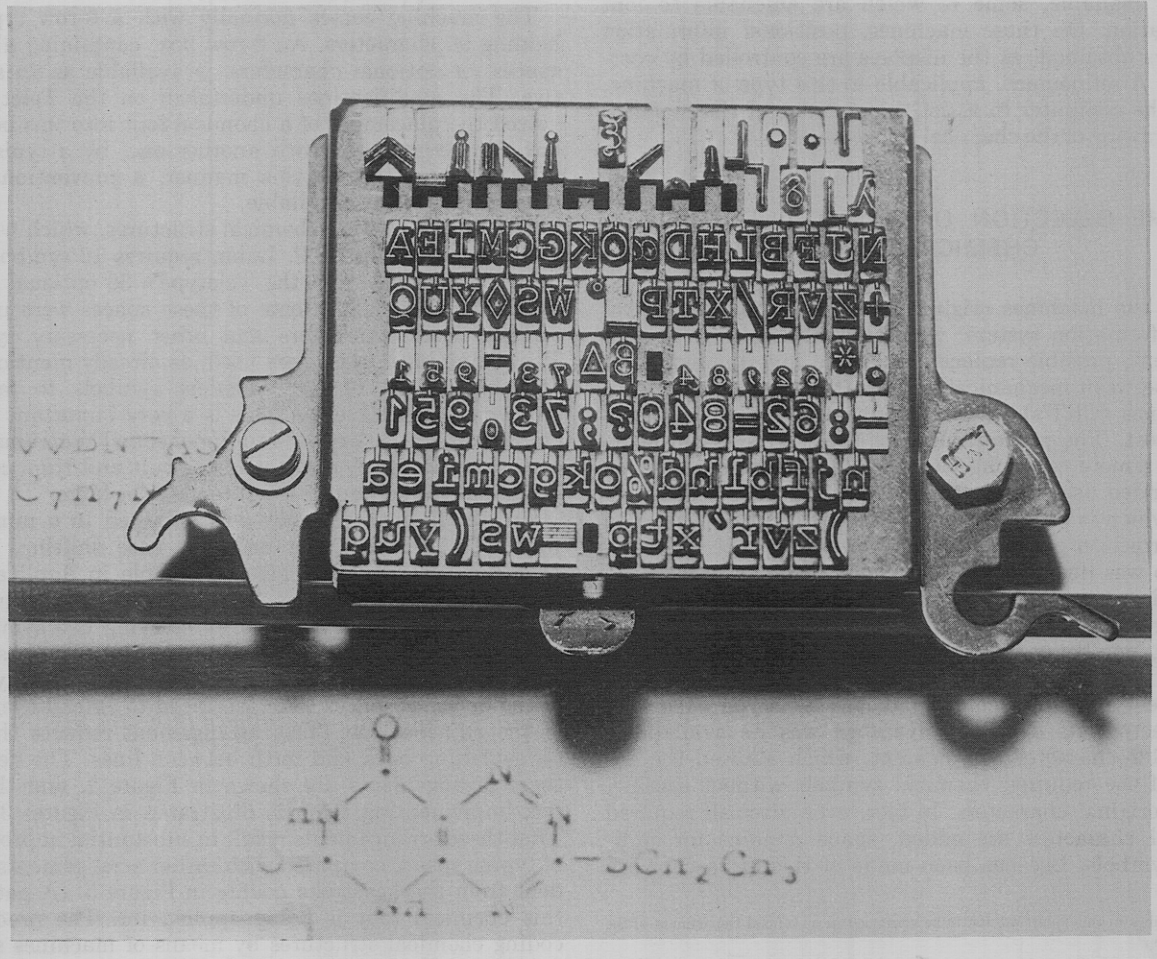

Figure 3. The 8-row type basket with chemical symbols

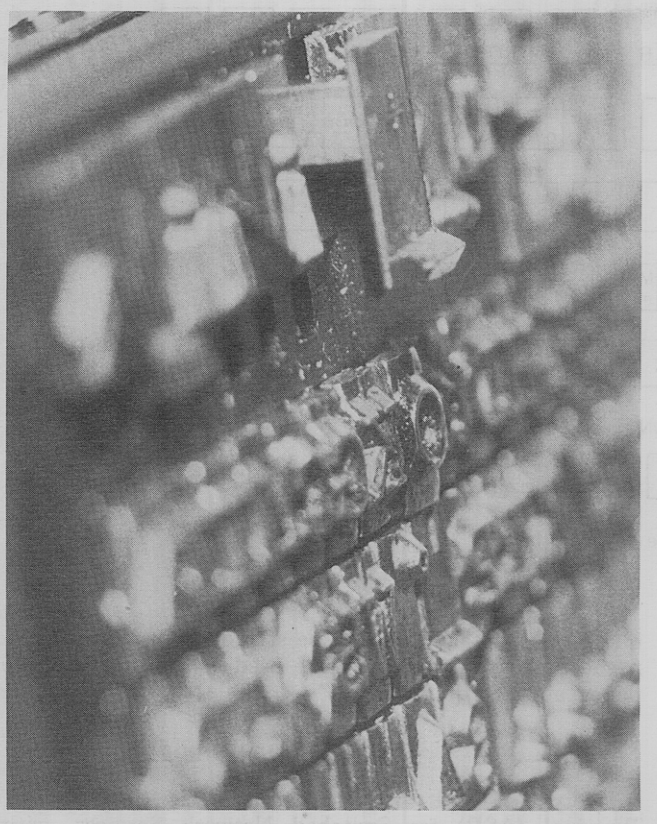

Figure 4. Detail of type basket, showing extended symbols overlapping a sacrificed space

tions. However, this modification was not adopted, even though tests showed a gain of 10–15% in the speed of structure typing. It was rejected because of its relatively high installation cost and because it would complicate subsequent maintenance.

Unlike the Mergenthalers, however, the teletypewriters can be connected to a magnetic tape unit, on which fre-

Structure to be typed	Keyboard used: Mullen[2]	Keyboard used: Feldman
		
Print keys used	12	12
Control keys used	13	7
Total keys used	25	19
		
Print keys used	12	11
Control keys used	21	7
Total keys used	33	18
		
Print keys used	11	11
Control keys used	11	8
Total keys used	22	19

Figure 5. Keystroke comparisons—Teletype *vs.* Mullen machine

Figure 6. View of Teletype keyboard

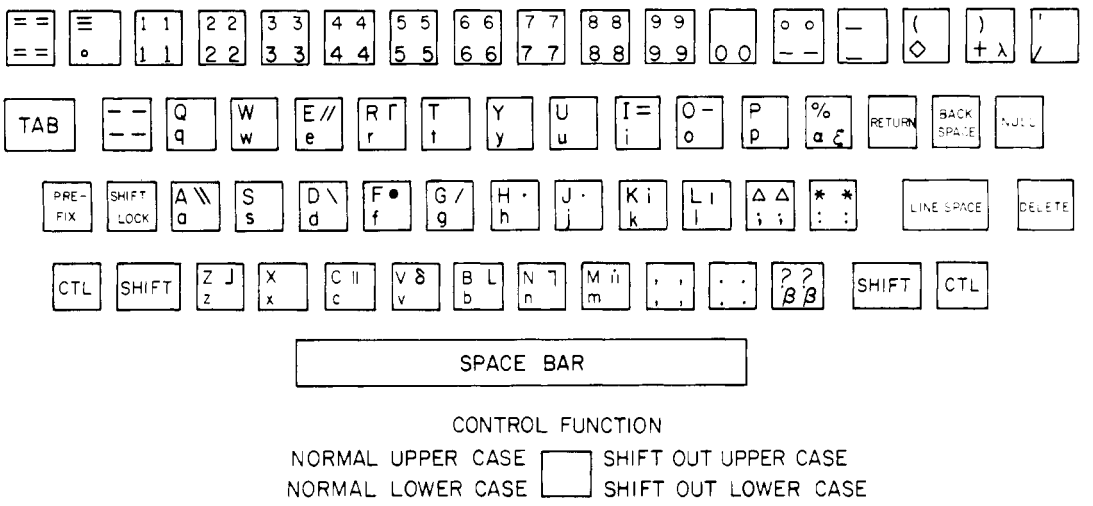

Figure 7. Teletype keyboard layout

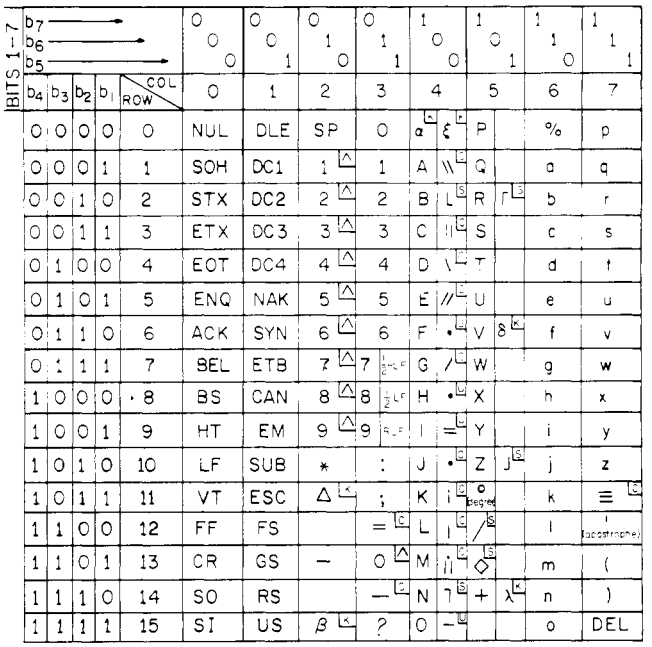

Figure 8. Teletype code chart

Abbreviations (with the exception of RLF = Reverse Line Feed) are according to the "Proposed American National Standard Names and Abbreviations for Identifying Control Character Keys on Keyboards Implementing the American National Standard Code for Information Interchange" (X4-A9/268C, April 10, 1971), available from the Computer Business Equipment Manufacturers Association, Washington, D. C. 20036

quently used fragments can be stored, to be typed out as needed. This unit may also be used as an alternative to paper tape recording.

SPECIFICATION

Teletype Model 37/302-3D Automatic Send-Receive Terminal (ASR) for Switched Network Services, with 8½-inch friction feed platen, wide table, keyboard overlay (visual aid), and 8-row "chemical" type box. Model 37/402-1D Punch and Reader (included in ASR code). Model 4210A-3AD Magnetic Tape Data Terminal, with Character Recognition Expander.

ACKNOWLEDGMENT

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LITERATURE CITED

(1) Feldman, A., Holland, D. B., and Jacobus, D. P., "The Automatic Encoding of Chemical Structures," *J. Chem. Doc.* **3,** 187 (1963).

(2) Mullen, J. M., "Atom-by-Atom Typewriter Input for Computerized Storage and Retrieval of Chemical Structures," *J. Chem. Doc.* **7,** 88 (1966).

(3) Feldmann, R. J., "An Application of Interactive Computing—A Chemical Information System," *J. Chem. Doc.* **12,** 41 (1972).

(4) Jacobus, D. P., Davidson, D. E., Feldman, A. P., and Schafer, J. A., "Experience with the Mechanized Chemical and Biological Information Retrieval System," *J. Chem. Doc.* **10,** 135 (1970).

(5) Ackerman, M. R., "Input-Output (I-O) Devices for the IDEEA Network," Memorandum Report **M 70-71-1,** Frankford Arsenal, Philadelphia, Pa., April 1970 (AD 870120 L).

(6) Holland, D. B., Jacobus, D. P., Feldman, A., and Moberly, B. R., "The Coordinate Concept," *Contr. Eng.* **11** (8), 60 (1964).